Supporting Information

Nickel-Catalyzed Diastereoselective Alkyl-Alkyl Kumada Coupling Reactions

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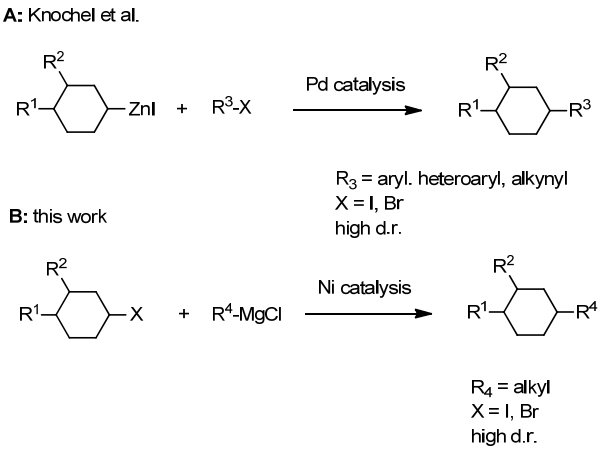
Scheme S1. Approaches to Diastereoselective Cross Coupling Reactions.



Experimental Section

1. Chemicals and Reagents

All manipulations were carried out under an inert N_2(g) atmosphere using standard Schlenk or glovebox techniques. Solvents were purified using a two-column solid-state purification system (Innovative Technology, NJ, USA) and transferred to the glove box without exposure to air. Deuterated solvents were purchased from Cambridge Isotope Laboratories, Inc., and were degassed and stored over activated 3 Å molecular sieves. Unless otherwise noted, all other reagents and starting materials were purchased from commercial sources and used without further purification. Liquid compounds were degassed by standard freeze-pump-thaw procedures prior to use. The following chemicals were prepared according to literature procedure: complex **1**,[1] complex **2**, 4-methylcyclohexyl iodide (**3a**), 3-methylcyclohexyl iodide (**3b**), 4-iodocyclohexanecarboxylate, 3-iodocyclohexanecarboxylate, [2], tetrahydropyran (**3c**),[3] tetrahydropyran (**3d**).[4]

2. Physical methods

The ^{1}H and ^{13}C NMR spectra were recorded at 293 K on a Bruker Avance 400 spectrometer. ^{1}H NMR chemical shifts were referenced to residual solvent as determined relative to Me_4Si (δ = 0 ppm). The $^{13}C\{^1H\}$ chemical shifts were reported in ppm relative to the carbon resonance of $CDCl_3$ (77.0 ppm). GC-MS measurements were conducted on a Perkin-Elmer Clarus 600 GC equipped with Clarus 600T MS. HRESI-MS measurements were conducted at the EPFL ISIC Mass Spectrometry Service with a Micro Mass QTOF Ultima spectrometer.

3. Determination of the diastereoisomeric ratios of starting materials and coupling products (Scheme 2).

- **Starting materials:**

The diastereoisomeric ratios of the substrates 4-methylcyclohexyl iodide and 3-methylcyclohexyl iodide were determined by ^{1}H NMR analysis. The analysis was based on the magnitude of the coupling of the signal corresponding to the geminal proton of the iodine (chemical shift between 4 and 5 ppm). In the case of 4-methylcyclohexyl iodide, the conformational analysis leads to conclusion that the *trans* isomer should have a multiplet and the *cis* isomer should have a singlet. In the case of 3-methylcyclohexyl iodide, the conformational analysis leads to the conclusion that the *cis* isomer should have a multiplet and the *trans* isomer should have a singlet. Figure S1 shows the ^{1}H NMR spectra of both substrates.

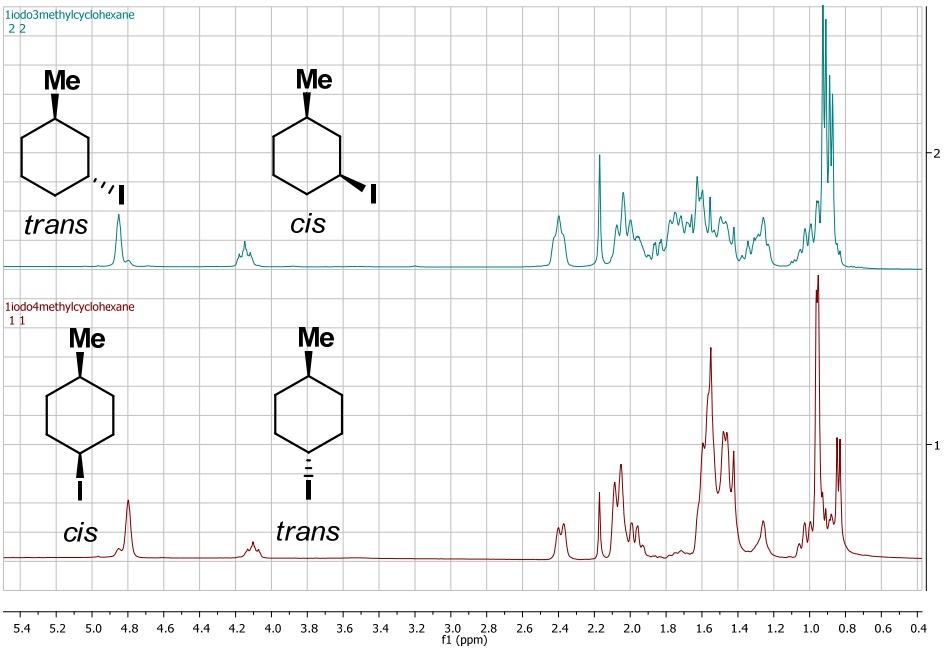


Figure S1. ^{1}H NMR spectra of the 3-methylcyclohexyl iodide (upper one) and of 4-methylcyclohexyl iodide (bottom one)

This information was useful for the identification of the diastereoisomers during the GC-MS analysis. Table S1 shows the comparison (and so the identification) of the diastereoisomeric ratios proportions obtained by integrations of GC signals and ^{1}H NMR signals.

Table S1. Identification of the signals corresponding to the diastereoisomers of each methylcyclohexyl iodide.

Substrate	**GC-MS**	**^{1}H NMR (H geminal with I)**
trans 4-methylcyclohexyl iodide	30	34
cis 4-methylcyclohexyl iodide	70	66
trans 3-methylcyclohexyl iodide	57	57
cis 3-methylcyclohexyl iodide	43	43

- **Coupling products:**

The diastereoisomeric ratios of the coupling products were determined by NMR techniques. The analysis of 1-butyl-4-methylcyclohexane and 1-butyl-3-methylcyclohexane is used as examples here. The literature[5] indicates that ^{1}H NMR shows separate and identifiable axial and equatorial proton resonances for the cyclohexane at low temperature. This indicates that the chemical environment is different for these protons: the axial protons are more electronically shielded because of the closer electronic densities of the other axial hydrogens. Anteunis *et al.*[6] have also shown that for mono-, di- and trimethylcyclohexanes, the difference between the chemical shifts of equatorial protons and axial protons of a same carbon ($\Delta\delta_{eq\text{-}ax}$) is bigger if they are next to an equatorial methyl substituent than if they are besides an axial methyl substituent. The signals corresponding to these protons can be easily identified by Heteronuclear Single Quantum Correlation NMR (HSQC). Figure S2 shows the identification of the *trans* (black dashed line) and *cis* (blue dashed line) isomers from the commercial available 1,4-dimethylcyclohexane (in a *trans*/*cis* mixture). The $\Delta\delta_{eq\text{-}ax}$ is around 0.75 ppm for the *trans* isomer and 0.15 ppm for the *cis* isomer. These results are consistent with the literature because the *trans* isomer has the methyl substituents preferentially on the equatorial position, giving a big $\Delta\delta_{eq\text{-}ax}$. On the other hand, the *cis* isomer has always one methyl on axial, giving a small $\Delta\delta_{eq\text{-}ax}$.

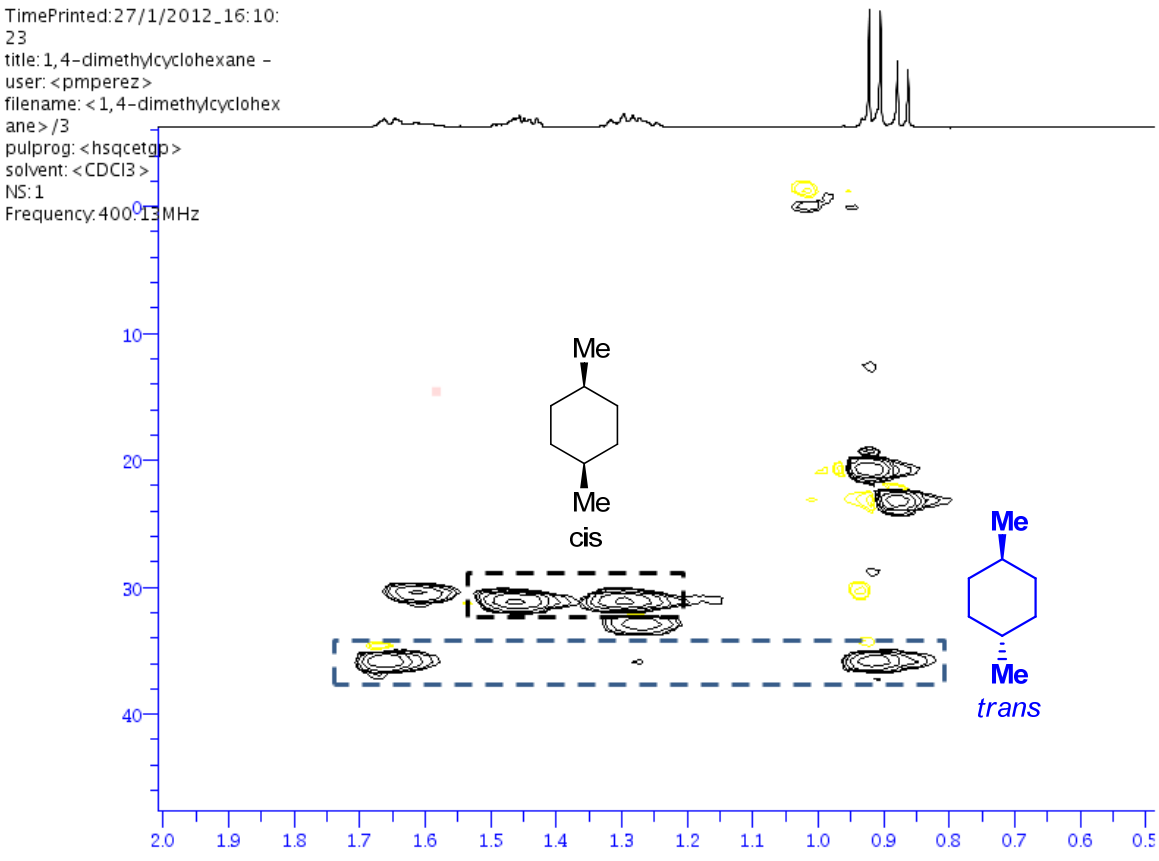


Figure S2. HSQC spectrum of commercial available 1,4-dimethylcyclohexane

The same analysis could be done for the cross-coupling product 1-butyl-4-methyl-cyclohexane. The HSQC spectrum of 1-butyl-4-methyl-cyclohexane obtained by using the

complex **2** as catalyst was used as a reference (Figure S3). The signals enclosed with the red dashed lines correspond to the geminal axial-equatorial protons of *cis* isomer, and the signals enclosed with the blue dashed lines correspond to *trans* isomer.

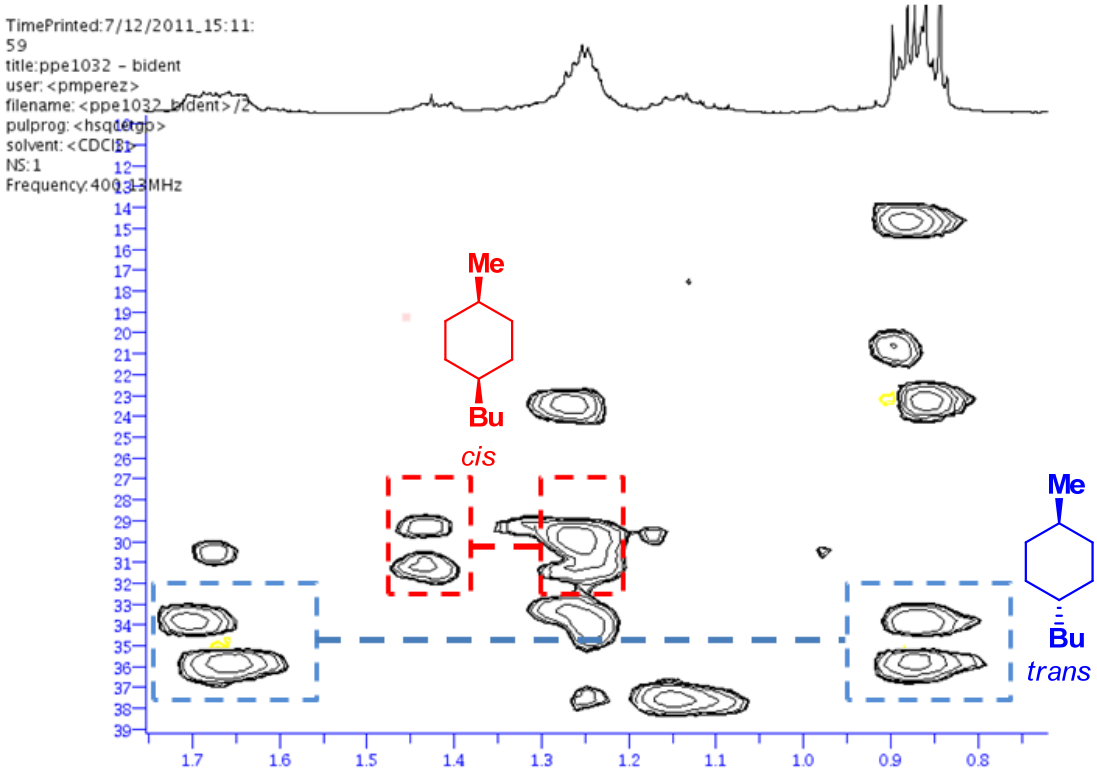


Figure S3. HSQC of cross-coupling product 1-butyl-4-methyl-cyclohexane obtained by catalysis with complex **2**

Once the signals of each diastereoisomer of 1-butyl-4-methyl-cyclohexane were identified, this information could be used to analyze the HSQC of the cross-coupling product obtained by catalysis with **1**. As it is shown in Figure S4, the coupled signals corresponding to *cis* isomer disappeared almost completely and only the signals of *trans* isomer were still strong observed. This leads to the conclusion that the major isomer is the *trans* one.

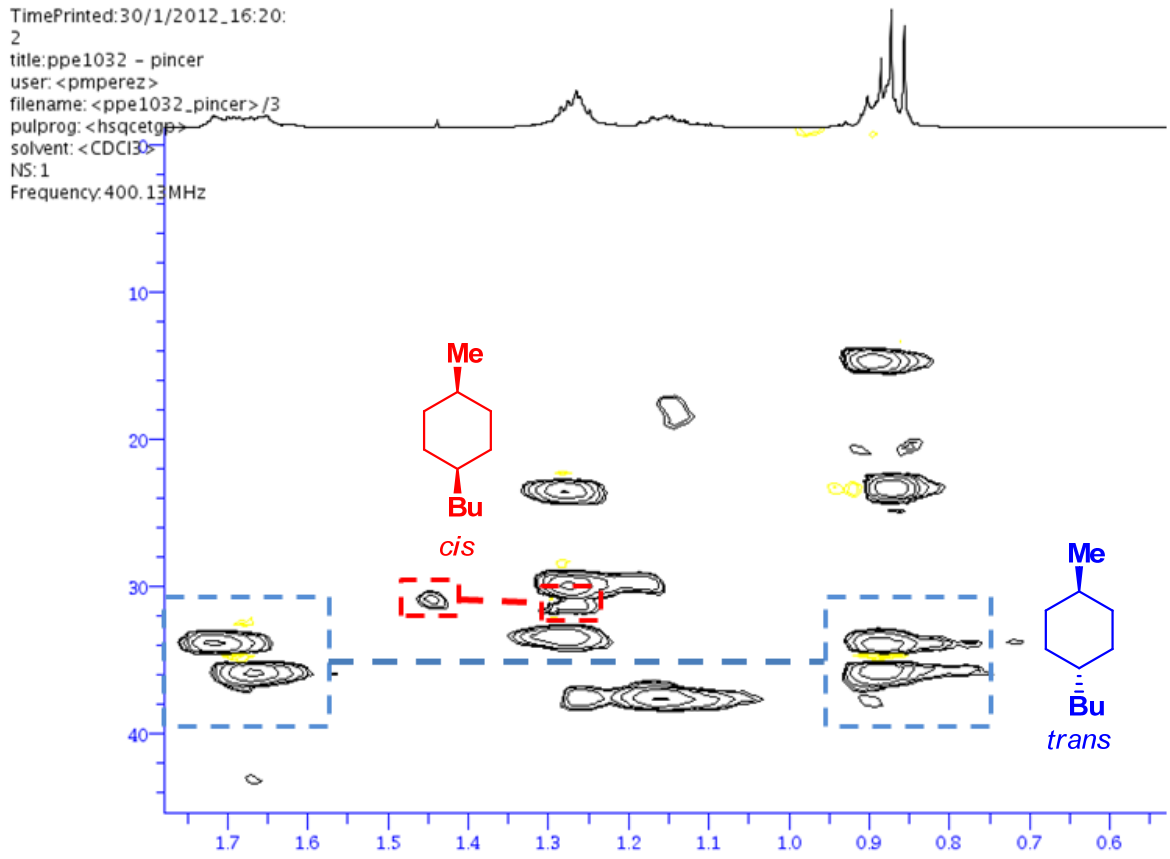


Figure S4. HSQC of cross-coupling product 1-butyl-4-methyl-cyclohexane obtained by catalysis with complex **1**

The stereoisomeric ratios of the 1,3- coupling products were deduced similarly by the ^{1}H NMR analysis. The NMR databases[7] of the 1,3dimethylcyclohexane show that the pure *cis* isomer have a highly shielded signal (compared to the pure *trans* isomer), around 0.5 ppm, corresponding to the axial hydrogen between the two methyl substituents. We propose that the low chemical shift of this proton is due to the electronic influence of the two methyl substituents pointing at the same direction. Figure S5 shows the ^{1}H NMR of the commercially available 1,3-dimethylcyclohexane (in a *cis*/*trans* mixture). It can be observed that the above mentioned signal (enclosed in the red dashed line) can be easily identifiable without any superposition with the *trans* isomer's spectrum.

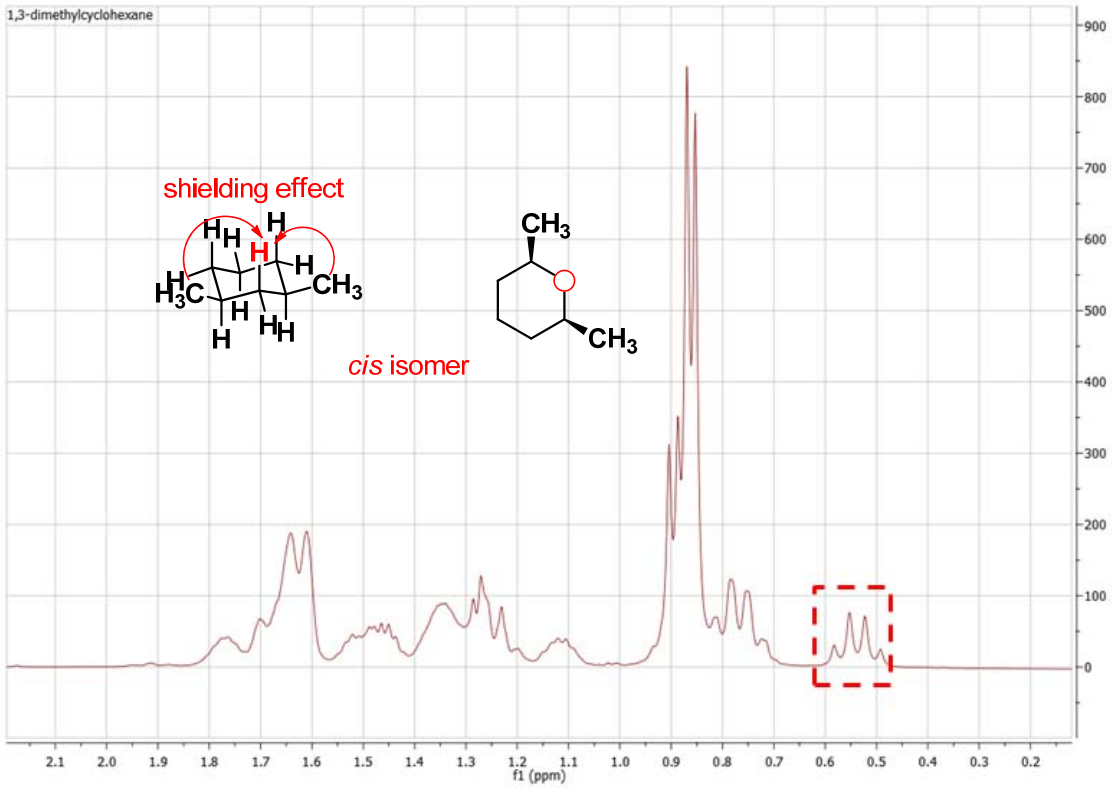


Figure S5. ^{1}H NMR spectrum of commercial available 1,3-dimethylcyclohexane

The ^{1}H NMR spectra (Figure S6) of the coupling product 1-butyl-3-methyl-cyclohexane produced by catalysis by **2** (green spectrum) and by **1** (red spectrum) show that this typical low chemical shift signal is conserved after the catalysis with **1**. Considering the high d.r. determined by GC-MS analysis, it can be unambiguously concluded that the major product for this reaction is the *cis* isomer.

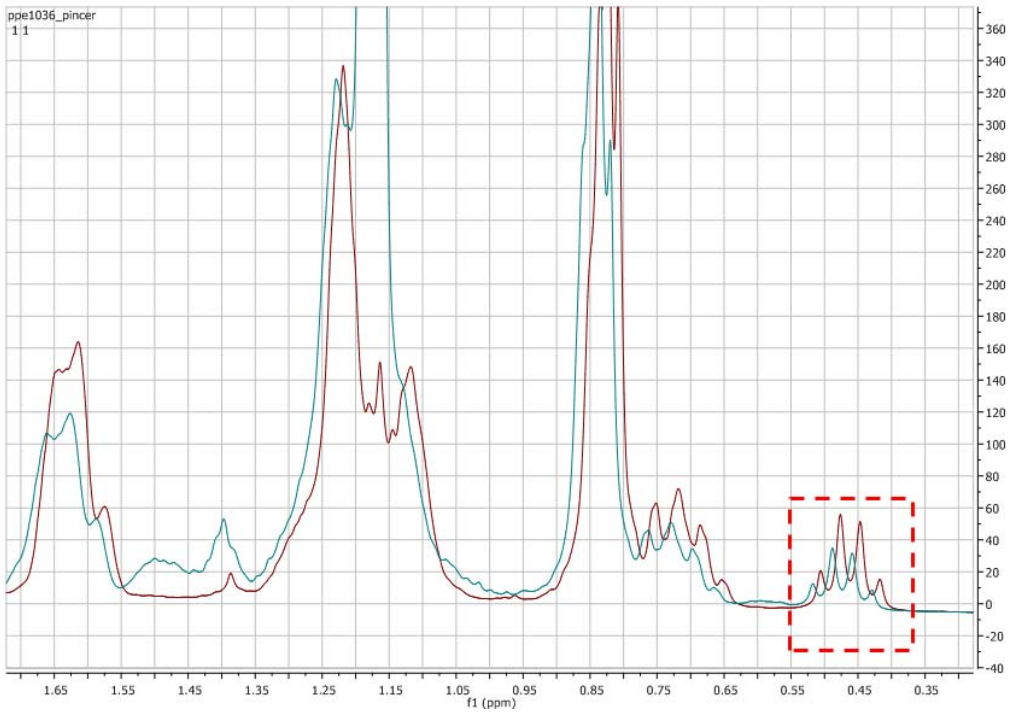


Figure S6. ^{1}H NMR spectra of the product 1-butyl-3-methyl-cyclohexane.

4. General procedures for Scheme 2 and Table 1

Standard conditions: A solution of alkyl-MgCl (commercially available, 0.6 mmol) was diluted to 3.5 mL with THF. The solution was then slowly added by the syringe pump over 2 h to a solution containing [(^{Me}N$_2$N)Ni-Cl] (15 mg, 0.043 mmol), 0.75 mL of DMA, and the iodide (0.5 mmol) at -20°C. After the addition, the solution was still stirred for 30 min at -20°C. It was then quenched by the addition of 5 mL of a saturated solution of NH_4Cl and 5 mL of water. The organic phase in the resulting solution mixture was extracted with ether (3 times, 10 mL each), dried over Na_2SO_4, filtered, and subject to GC analysis. 60 µL of decane (0.31 mmol) was used as an internal standard.

Note for TEMPO-test

The coupling reaction of ^{n}Bu-MgCl with 4-methylcyclohexyl iodide and with 3-methylcyclohexyl iodide were also conducted in the presence of one equivalent of a radical inhibitor ((2,2,6,6-tetramethylpiperidin-1-yl)oxidanyl, TEMPO). The yield of the reaction decreased to 47 % and 46 %, respectively. However the d.r. of the coupling products were exactly the same as given in Scheme 2.

Note for the entries 15, 16, 17 and 18

The standard conditions were applied, with the change that the addition and reaction were carried out at room temperature.

Note for the entries 4, 5, 9, 10

Modified conditions: A solution of alkyl-MgCl or aryl-MgCl (commercially available, 0.6 mmol) was diluted to 3.5 mL with THF. The solution was then slowly added by the syringe pump over 2 h to a solution containing [(^{Me}N$_2$N)Ni-Cl] (15 mg, 0.043 mmol), 1 mL of THF, TMDEA (25 μL, 0.17 mmol), and the iodide or bromide (0.5 mmol) at -20 ^{o}C. After the addition, the solution was still stirred for 30 min at r.t. It was then quenched by the addition of 5 mL of a saturated solution of NH_4Cl and 5 mL of water. The organic phase in the resulting solution mixture was extracted with ether (3 times, 10 mL each), dried over Na_2SO_4, filtered, and subject to GC analysis. 60 μL of decane (0.31 mmol) was used as an internal standard.

Note for the entries 19 and 20

The modified conditions were applied, with the change that the addition and reaction were carried out at room temperature.

Note for entries 4, 5, 9, 10, 11, 12, 13, 14

These reactions were subjected to the isolation of the coupling products; the yields were therefore isolated yields.

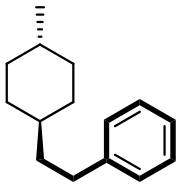
Note for entry 21

The d.r. of the starting material was determined by ^{1}H NMR analysis (55:45, *cis*:*trans*). It must be considered that in a cyclopentane system, the energetic difference between an "equatorial" substituent and an "axial" substituent is small, which leads to a low d.r. of the coupling product.

Determination of the d.r. value

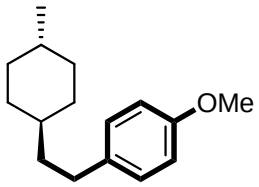
The determination of the d.r. values were made by GC-MS analysis (except for entries 13, 14, 17 and 18 for where the d.r. values were determined by ^{1}H NMR analysis).

5. Characterization of entries of table 1.

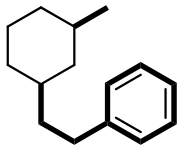


Entry 4
Purified by column (SiO_2, Hexane), 65% yield as a transparent liquid.
^{1}H NMR (400 MHz, $CDCl_3$): 7.36-7.26 (m, 2H), 7.25-7.16 (m, 3H), 2.65 (t, J = 8 Hz, 2H), 1.82-1.62 (m, 4H), 1.52-1.42 (m, 2H), 1.35-1.10 (br, 2H), 1.02-0.8 (m, 7H).

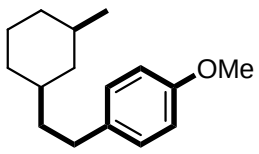
^{13}C NMR (100 MHz, $CDCl_3$): 143.2, 128.4, 128.3, 125.4, 39.3, 37.0, 35.3, 33.4, 33.3, 32.8, 22.8.
MS-APPI: calculated for ($C_{15}H_{22}$, M), 212.17160; found, 212.17177.
Anal. Calcd. C, 89.0; H, 11.0; Found: C, 89.2; H, 10.9.



Entry 5
Purified by column (SiO_2, Hexane:EtOAc 50:1), 81% yield as a transparent liquid.
^{1}H NMR (400 MHz, $CDCl_3$): 7.10 (d, *J* = 8 Hz, 2H), 6.83 (d, *J* = 8.4 Hz, 2H), 3.80 (s, 3H), 2.57 (t, *J* = 7.6 Hz, 2H), 1.85-1.75 (m, 4H), 1.60-1.50 (m, 2H), 1.40-1.15 (br, 2H), 1.05-0.8 (m, 7H).
^{13}C NMR (100 MHz, $CDCl_3$): 157.5, 135.3, 129.2, 113.7, 55.3, 39.6, 37.0, 35.3, 33.3, 32.9, 32.4, 22.8.
HRESI-MS: calculated for ($C_{16}H_{25}O$, M+H), 233.1905; found, 213.1886
Anal. Calcd. C, 82.7; H, 10.4; Found: C, 82.4; H, 10.2.

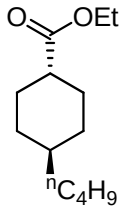


Entry 9
Purified by column (SiO_2, Hexane), 79% yield as a transparent liquid.
^{1}H NMR (400 MHz, $CDCl_3$): 7.37-7.30 (m, 2H), 7.28-7.20 (m, 3H), 2.70 (t, *J* = 8 Hz, 2H), 1.90-1.70 (m, 4H), 1.62-1.50 (m, 2H), 1.45-1.3 (br, 3H), 1.00-0.8 (m, 5H), 0.70-0.60 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): 143.2, 128.4, 128.3, 125.6, 42.3, 39.7, 37.4, 35.4, 33.3, 33.0, 32.7, 26.4, 23.1.
MS-APPI: calculated for ($C_{15}H_{22}$, M), 212.17160; found, 212.17167.

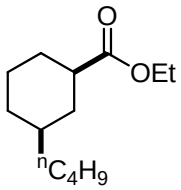


Entry 10
Purified by column (SiO_2, Hexane:EtOAc 50:1), 69% yield as a transparent liquid.
^{1}H NMR (400 MHz, $CDCl_3$): 7.10 (d, *J* = 8 Hz, 2H), 6.82 (d, *J* = 7.6 Hz, 2H), 3.79 (s, 3H), 2.57 (t, *J* = 8 Hz, 2H), 1.80-1.62 (m, 4H), 1.52-1.42 (m, 2H), 1.36-1.16 (br, 3H), 0.95-0.75 (m, 5H), 0.65-0.50 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): 157.5, 135.3, 129.2, 113.7, 55.2, 42.3, 39.8, 37.2, 35.4, 32.8, 32.6, 32.2, 26.2, 23.0.
HRESI-MS: calculated for ($C_{16}H_{25}O$, M+H), 233.1905; found, 213.1927

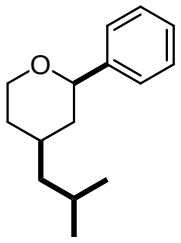
Anal. Calcd. C, 82.7; H, 10.4; Found: C, 83.1; H, 10.2



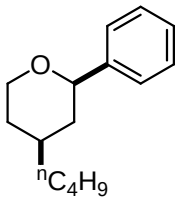
Entry 11
Purified by column (SiO_2, Hexane:EtOAc 50:1), 74% yield as a transparent liquid.
^{1}H NMR (400 MHz, $CDCl_3$): 4.17-4.07 (m, 2H), 2.20 (t, *J* = 12 Hz, 1H), 1.95 (d, *J* = 12 Hz, 2H), 1.80 (d, *J* = 12 Hz, 2H), 1.59-1.45 (m, 1H), 1.43-1.32 (m, 2H), 1.30-1.10 (m, 10H), 0.98-0.82 (m, 4H).
^{13}C NMR (100 MHz, $CDCl_3$): 176.2, 60.0, 43.6, 37.0, 37.0, 32.3, 29.1, 29.0, 23.0, 14.2, 14.1.
HRESI-MS: calculated for ($C_{13}H_{25}O_2$, M+H), 213.1855; found, 213.1865.



Entry 12
Purified by column (SiO_2, Hexane:EtOAc 50:1), 52% yield as a transparent liquid.
^{1}H NMR (400 MHz, $CDCl_3$): 4.15-4.05 (m, 2H), 2.26 (t, *J* = 9.6 Hz, 1H), 2.00-1.90 (m, 2H), 1.82-1.65 (m, 2H), 1.35-1.15 (m, 12H), 1.10-0.95 (m, 1H), 0.93-0.78 (m, 4H).
^{13}C NMR (100 MHz, $CDCl_3$): 176.2, 60.1, 43.6, 37.0, 37.0, 35.6, 32.5, 29.1, 29.0, 25.5, 23.0, 14.3, 14.1.
HRESI-MS: calculated for ($C_{13}H_{25}O_2$, M+H), 213.1855; found, 213.1865.



Entry 13
Purified by column (SiO_2, Hexane:EtOAc 50:1), 80% yield as a transparent liquid.
^{1}H NMR (400 MHz, $CDCl_3$): 7.44-7.17 (m, 5H), 4.30 (d, *J* = 11.2 Hz, 1H), 4.19-4.13 (m, 1H), 3.61 (t, *J* = 11.2 Hz, 1H), 1.93-1.51 (m, 4H), 1.41-1.10 (m, 4H), 0.89 (t, *J* = 4.8 Hz, 6H).
^{13}C NMR (100 MHz, $CDCl_3$): 143.2, 128.4, 127.4, 125.9, 80.0, 68.6, 46.5, 41.2, 33.3, 32.9, 24.3, 22.9, 22.84.
HRESI-MS: calculated for ($C_{15}H_{23}O$, M+H), 219.1749; found, 219.1750.



Entry 14
Purified by column (SiO_2, Hexane:EtOAc 50:1), 65% yield as a transparent liquid.
^{1}H NMR (400 MHz, $CDCl_3$): 7.44-7.17 (m, 5H), 4.32 (d, *J* = 10.8 Hz, 1H), 4.25-4.1 (m, 1H), 3.60 (t, *J* = 12 Hz, 1H), 1.95 (m, *J* = 12 Hz, 1H), 1.80-1.57 (m, 2H), 1.43-1.15 (m, 8H), 0.95-0.84 (m, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 143.3, 128.3, 127.3, 125.9, 80.0, 68.6, 41.1, 36.8, 35.7, 32.8, 28.7, 22.9, 14.2.
HRESI-MS: calculated for ($C_{15}H_{23}O$, M+H), 219.1749; found, 219.1750.

6. General procedure and source data for Figure 1.

For a more accurate quantification of the 3-methylcyclohexyl iodide in the reaction mixture, a calibration curve (Figure S7) was made using decane as internal standard (0.31 mmol). The curve is composed by: a vertical axis that represents the proportion of the GC signal areas (iodide-standard) and a horizontal axis that represents the proportion between the molar quantities (iodide-standard).

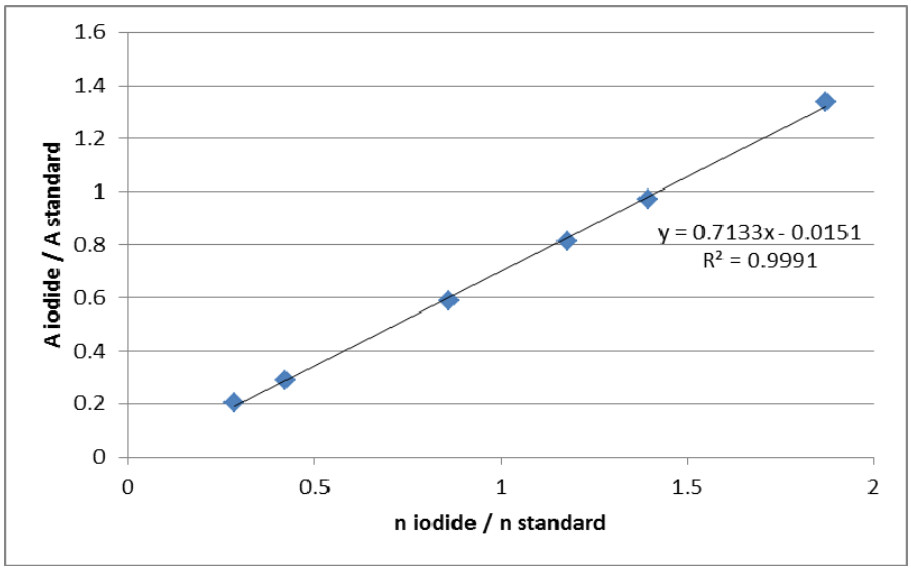


Figure S7. Calibration curve for the 3-methylcyclohexyl iodide.

Reaction profile (Figure 1, Top)

A 2 M solution of ^{n}Butyl-MgCl (commercially available, 0.6 mmol) was diluted to 3.5 mL with THF. The solution was then slowly added by the syringe pump (programmed for a total time of addition of 1 h) to a solution containing [($^{Me}N_2N$)Ni-Cl] (15 mg, 0.043 mmol), 0.75 mL of DMA, 60 µL of decane as internal standard (0.31 mmol) and the 3-methylcyclohexyl iodide (0.5 mmol) at -20°C. Small aliquots of the reaction mixture were taken each 5 minutes during the first 25 minutes of the addition. Each one of the aliquots was quenched with acetonitrile and analyzed then by GC-MS. Table S2 shows the results.

Table S2. Results for the construction of the reaction profile

	3-methylcyclohexyl iodide			***cis*-1-butyl-3-methylcyclohexane**
Time [sec]	***cis* isomer [mmol]**	***trans* isomer[mmol]**	**Total [mmol]**	**[mmol]**
0	0.227	0.304	0.530	0.000
5	0.296	0.157	0.452	0.036
10	0.243	0.085	0.328	0.114
15	0.238	0.072	0.310	0.161
20	0.176	0.041	0.216	0.216
25	0.125	0.020	0.146	0.261

Kinetic profile (Figure 1, Bottom)

A 2 M solution of ^{n}Butyl-MgCl (commercially available, 0.6 mmol) was diluted to 3.5 mL with THF. The solution was then one time added to a solution containing [($^{Me}N_2N$)Ni-Cl] (15 mg, 0.043 mmol), 2.25 mL of DMA, 60 µL of decane as internal standard (0.31 mmol), 7 mL of THF and the 3-methylcyclohexyl iodide (0.5 mmol) at -20°C. Small aliquots of the reaction mixture were taken each 20 seconds, leading to a total of 10 samples. Each one of the aliquots was quenched with acetonitrile and analyzed then by GC-MS. Table S3 shows the results.

Table S3. Results for the construction of the kinetic profile

	3-methylcyclohexyl iodide			***cis*-1-butyl-3-methylcyclohexane**
Time [sec]	***cis* isomer [mmol]**	***trans* isomer[mmol]**	**Total [mmol]**	**[mmol]**
0	0.120	0.397	0.516	0.000
20	0.146	0.320	0.466	0.017
40	0.167	0.289	0.456	0.030
60	0.175	0.251	0.427	0.038
80	0.184	0.233	0.417	0.048
100	0.195	0.216	0.411	0.056
120	0.204	0.205	0.409	0.064
140	0.205	0.190	0.395	0.071
160	0.198	0.175	0.373	0.074

180	0.204	0.167	0.372	0.081
200	0.207	0.159	0.366	0.087

Test for a possible role of $MgBr_2$ and NaI in the isomerization

The same conditions described for the general procedure were used to run two separated tests, replacing the Grignard reagent by stoichiometric quantities of anhydrous NaI and anhydrous $MgBr_2$ respectively. The reaction mixtures were stirred during 2 hours at -20°C. The goal of these reactions was to probe whether the isomerization reaction was mediated or catalyzed by a magnesium salt or an iodide salt. There was no isomerization observed for both tests. This result indicated that the isomerization required the nickel catalyst.

7. References

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[2] P. Ren, O. Vechorkin, K. von Allmen, R. Scopelliti, X. L. Hu, *J. Am. Chem. Soc*. **2011**, *133*, 7084-7095.

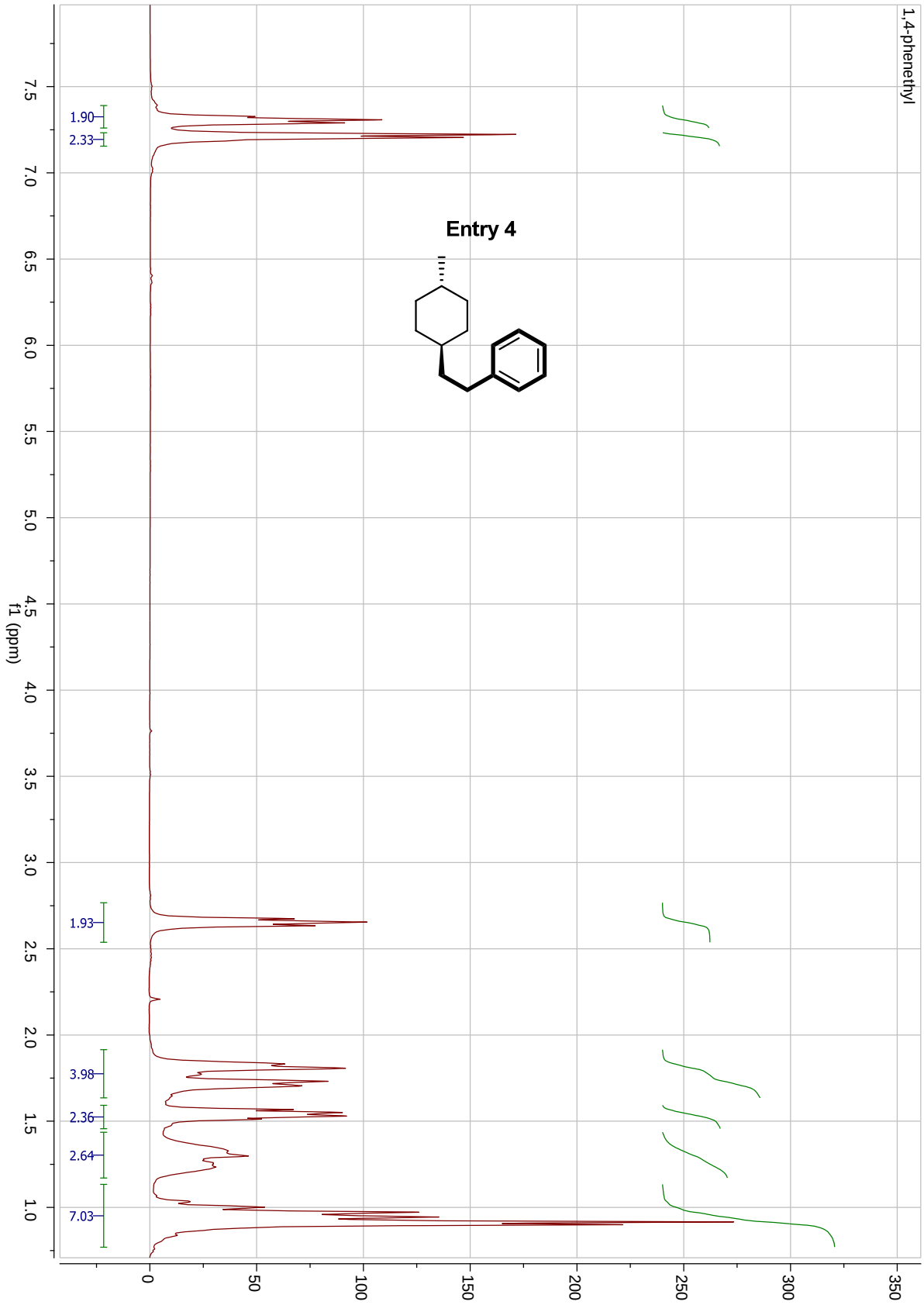
[3] G. Sabitha, K. B. Reddy, G. S. K. K. Reddy, N. Fatima, J. S. Yadav, *Synlett* **2005**, 2347-2351.

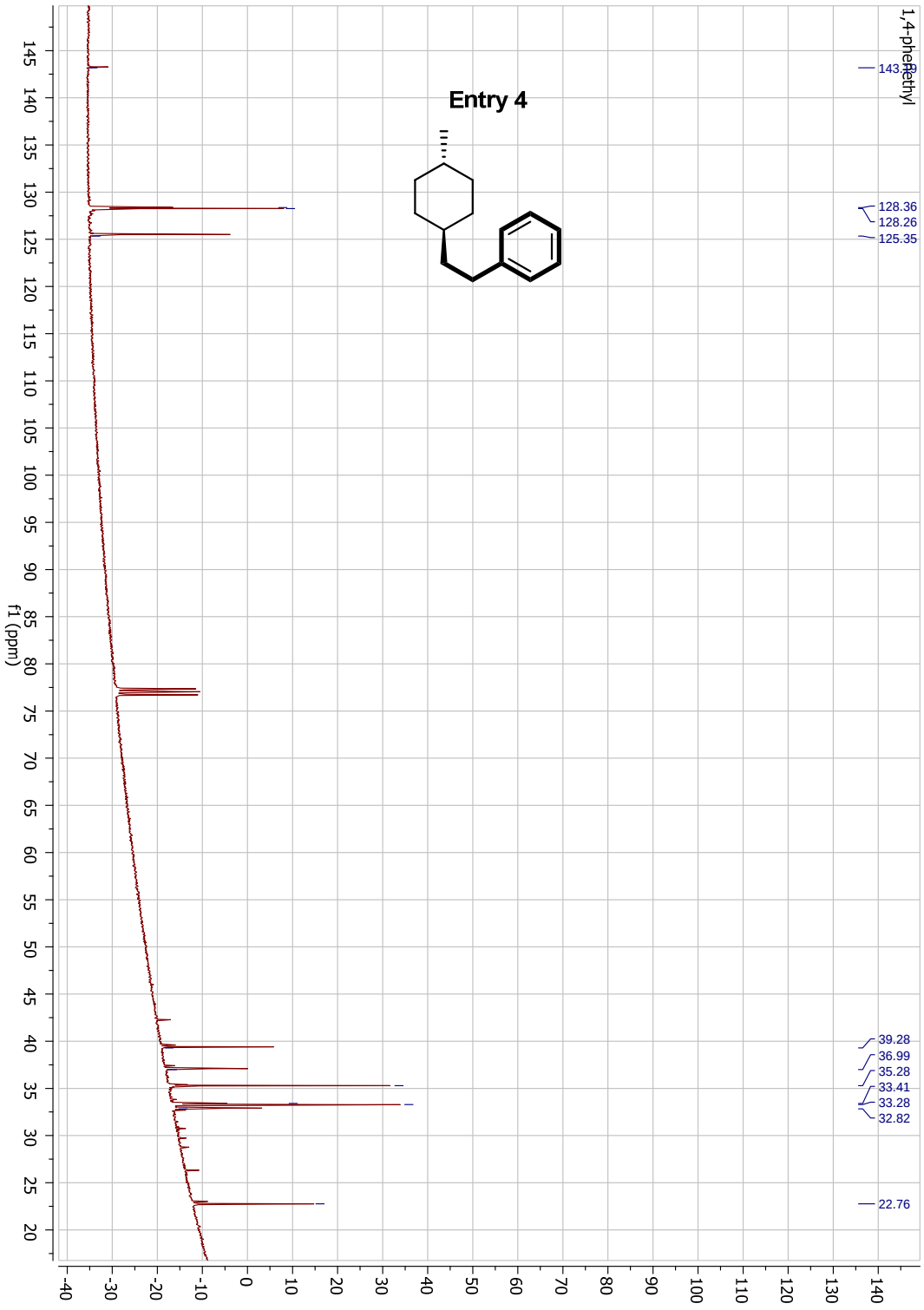
[4] D. Clarisse, B. Pelotier, O. Piva, F. Fache, *Chem. Comm.* **2012**, *48*, 157-159.

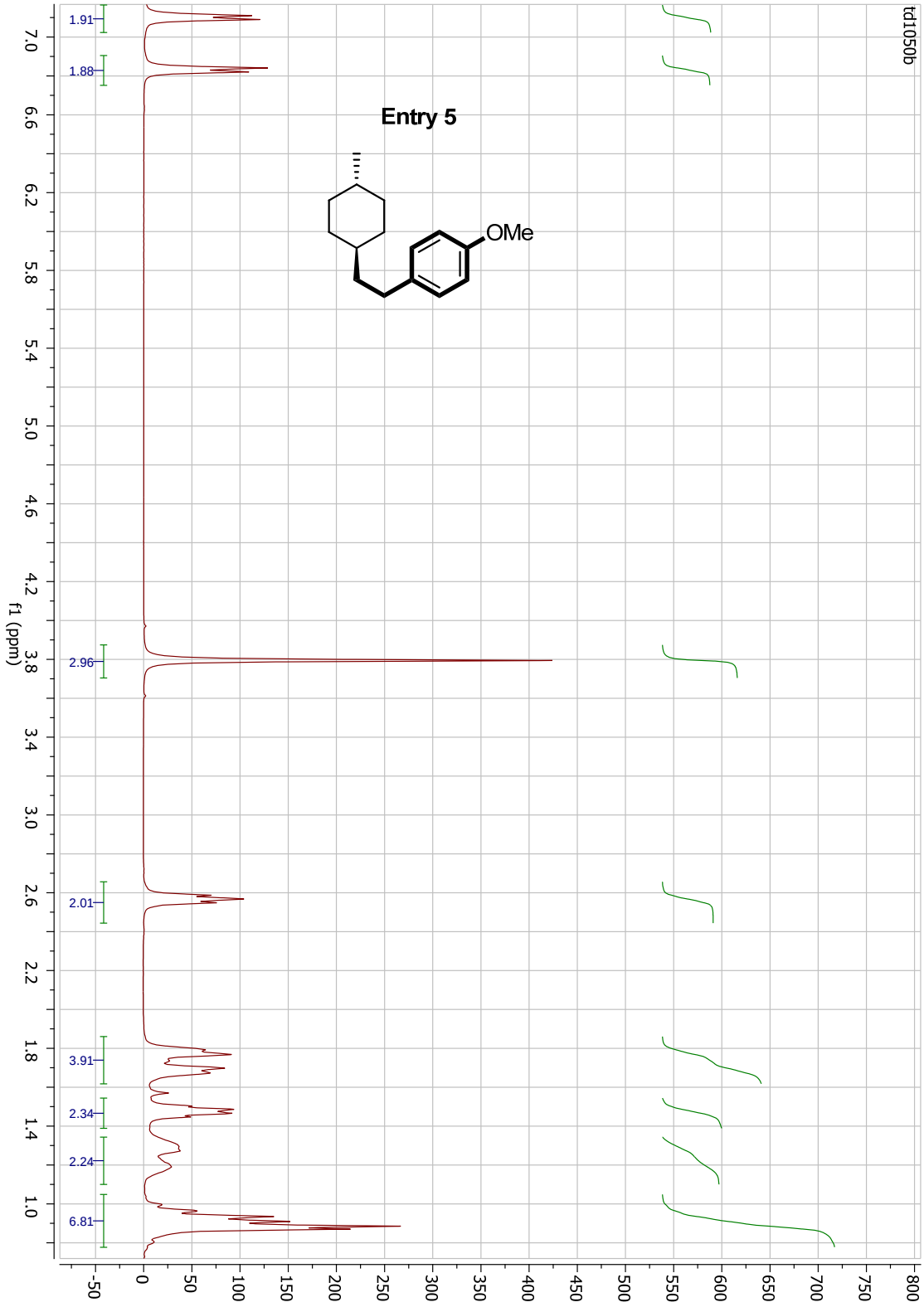
[5] F. R. Jensen, D. S. Noyce, C. H. Sederholm, A. J. Berlin, *J. Am. Chem. Soc.* **1962**, *84*, 386-389.

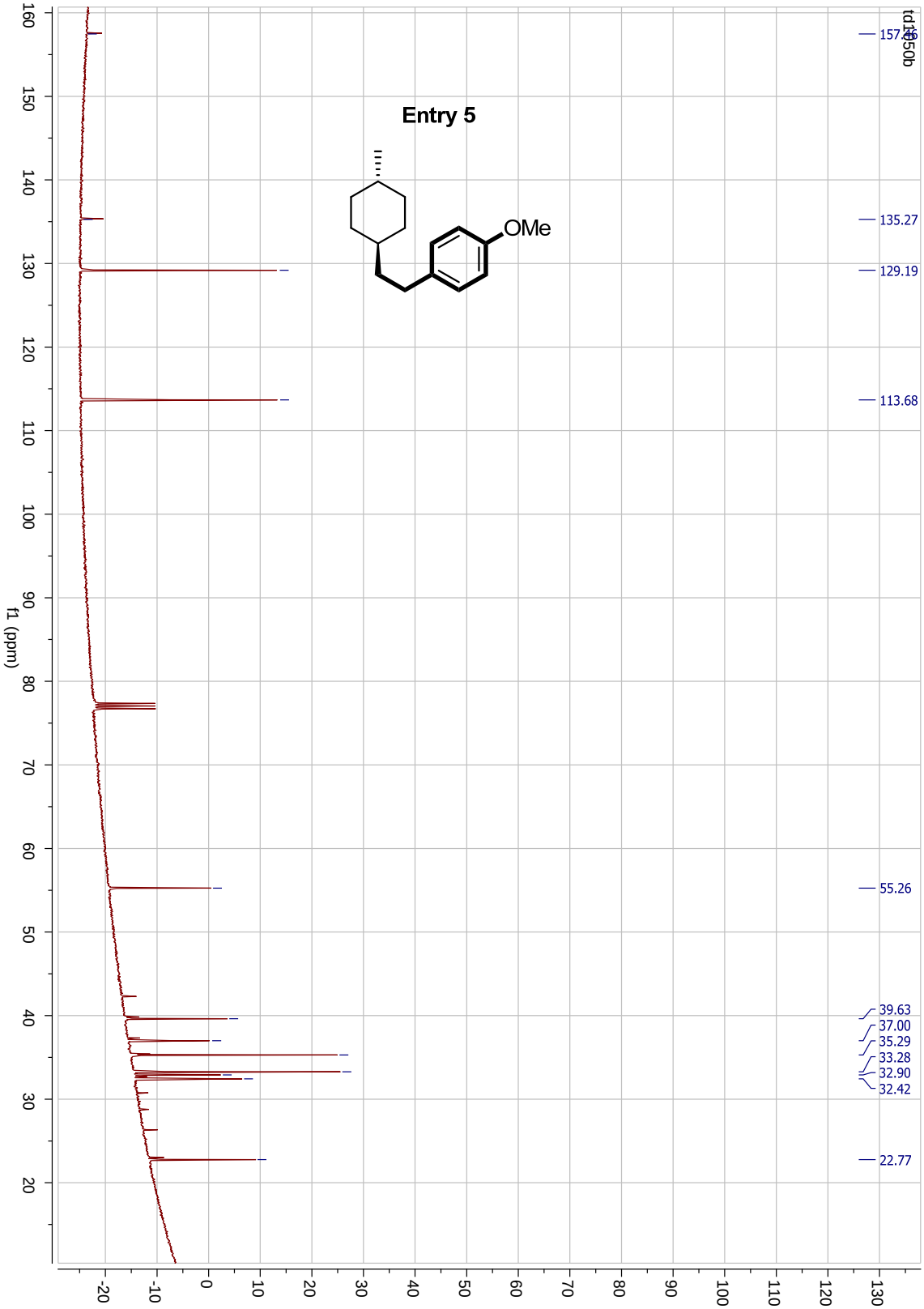
[6] D, Danneels, M. Anteunis, *Organic Magnetic Resonance* **1974**, *6*, 617-621.

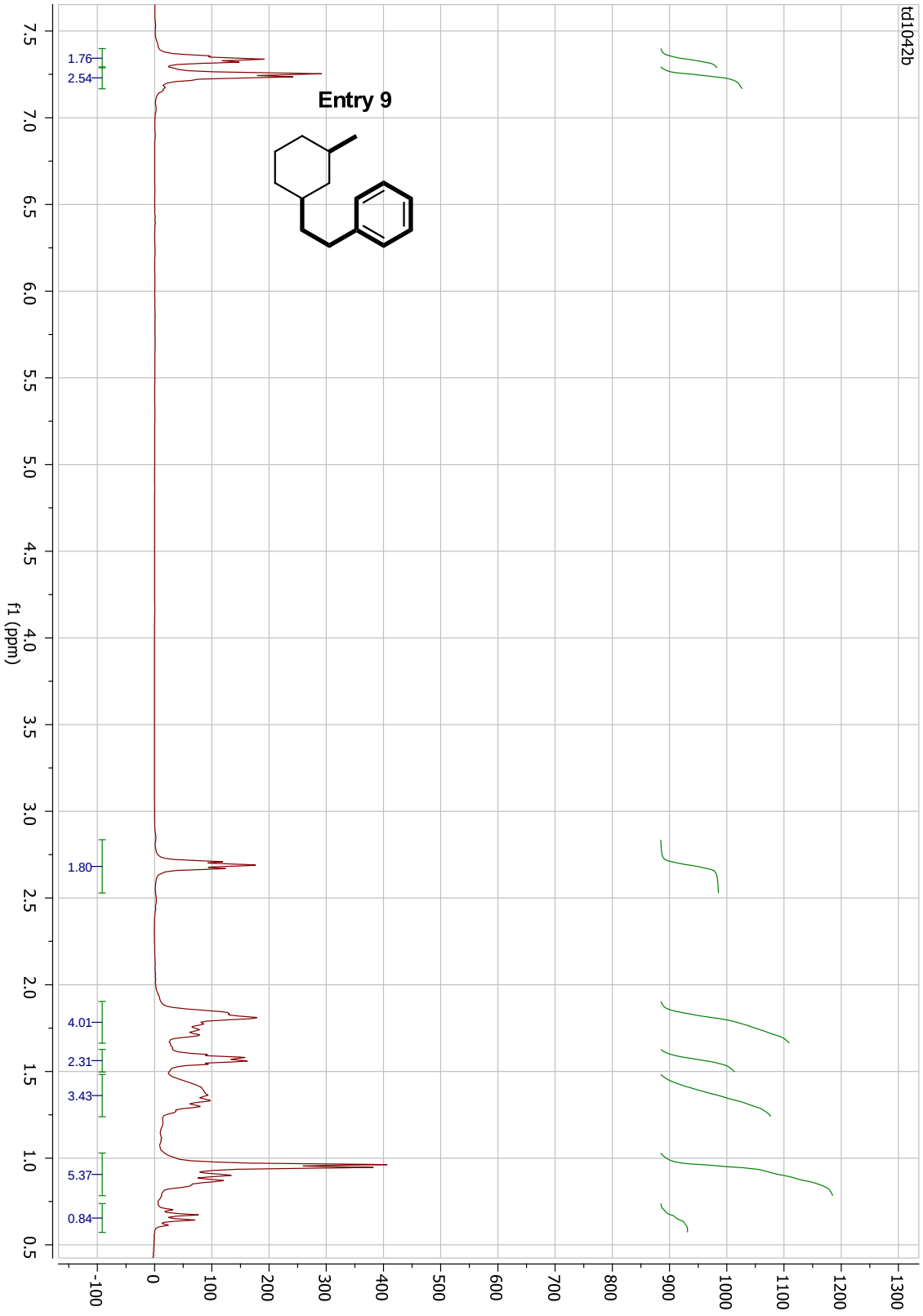
[7] SPECTRAL DATABASE FOR ORGANIC COMPOUNDS, SDBS.


1.4-phenethyl
Entry 4
1.90
2.33
1.93
3.98
2.36
2.64
7.03
f1 (ppm)


Entry 4
1,4-phenethyl
143.82
128.36
128.26
125.35
39.28
36.99
35.28
33.41
33.28
32.82
22.76
f1 (ppm)


td1050b
Entry 5
OMe
1.91
1.88
2.96
2.01
3.91
2.34
2.24
6.81
f1 (ppm)


Entry 5
OMe
td150b
157.
135.27
129.19
113.68
55.26
39.63
37.00
35.29
33.28
32.90
32.42
22.77
f1 (ppm)


td1042b
Entry 9
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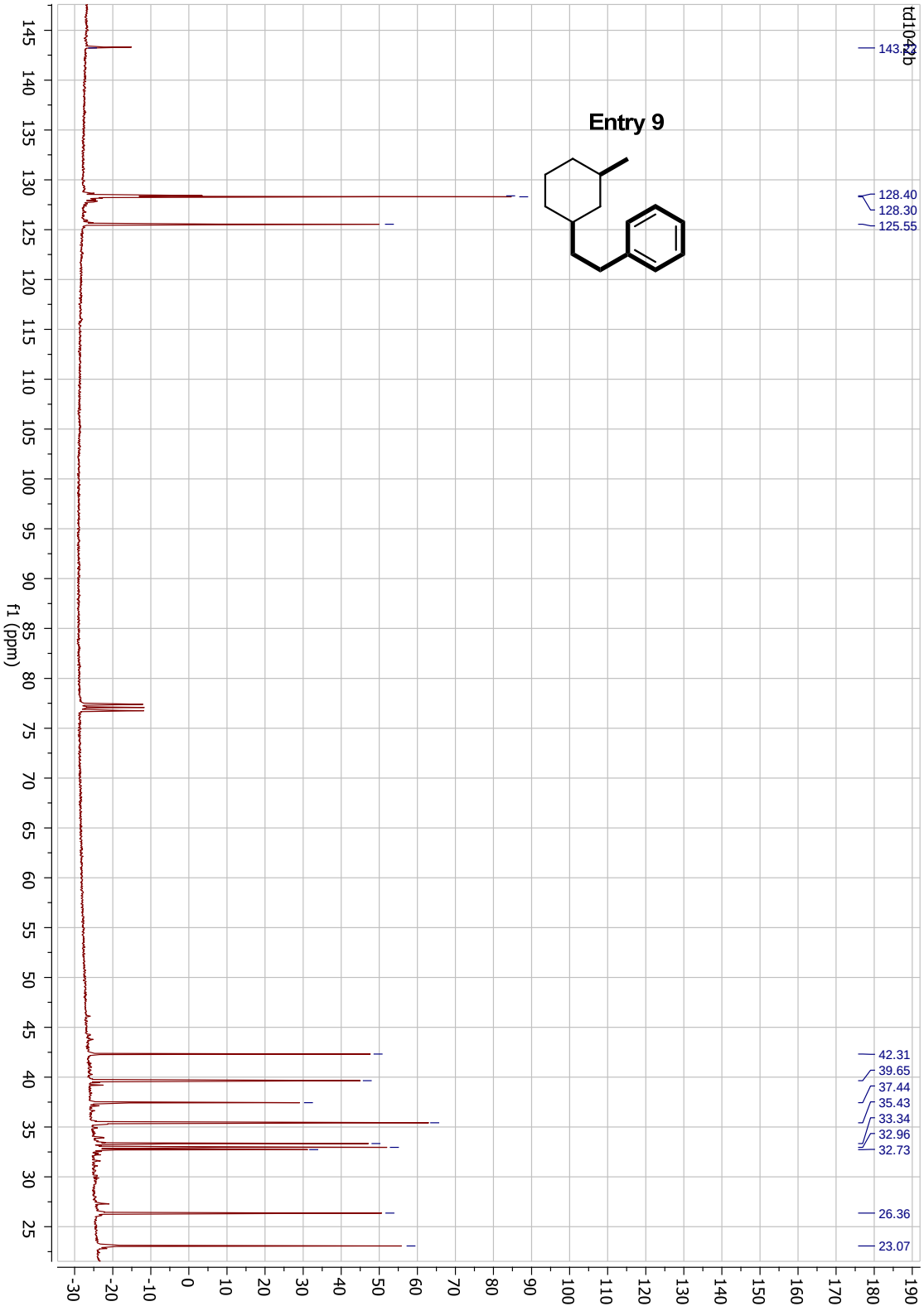
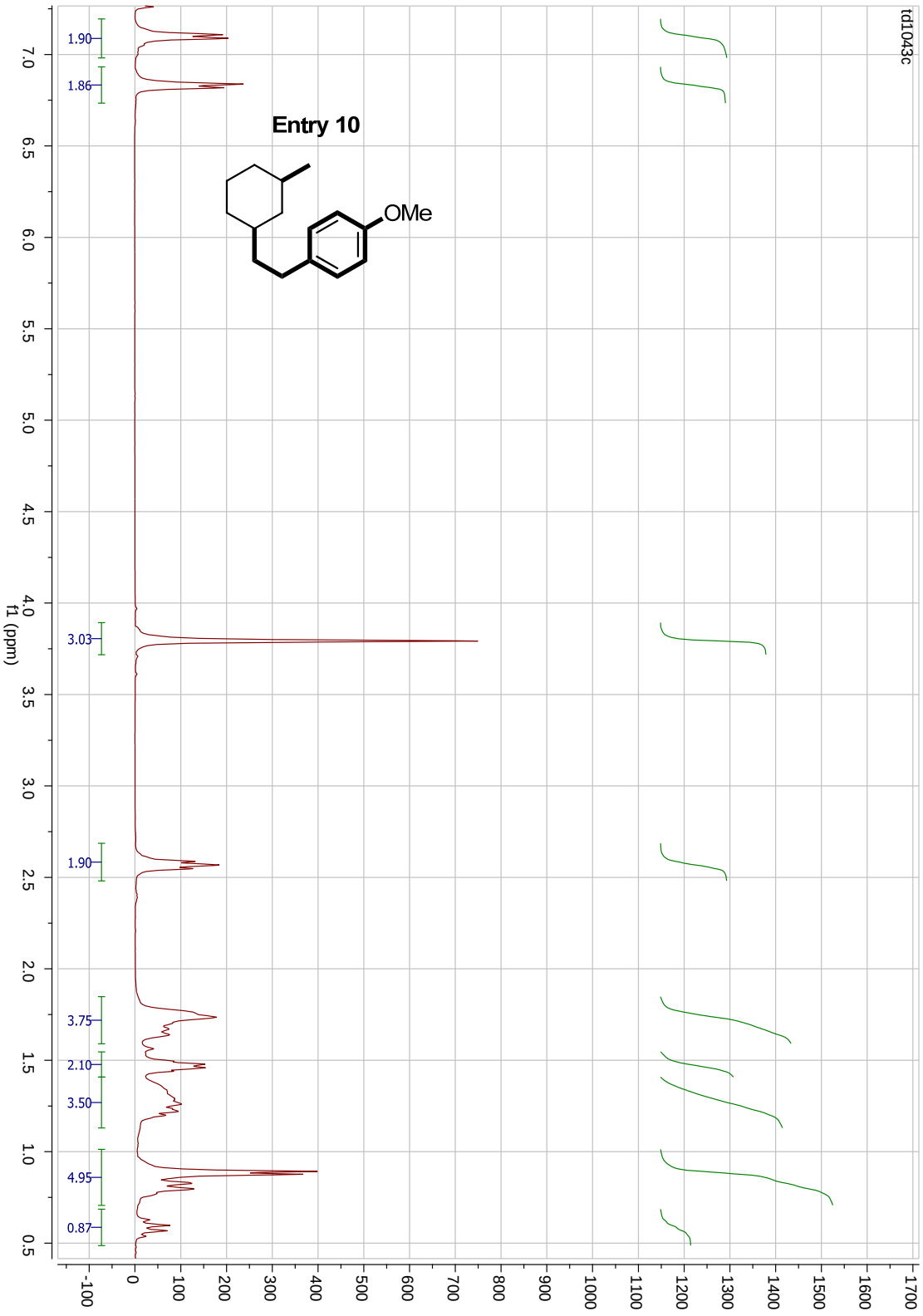
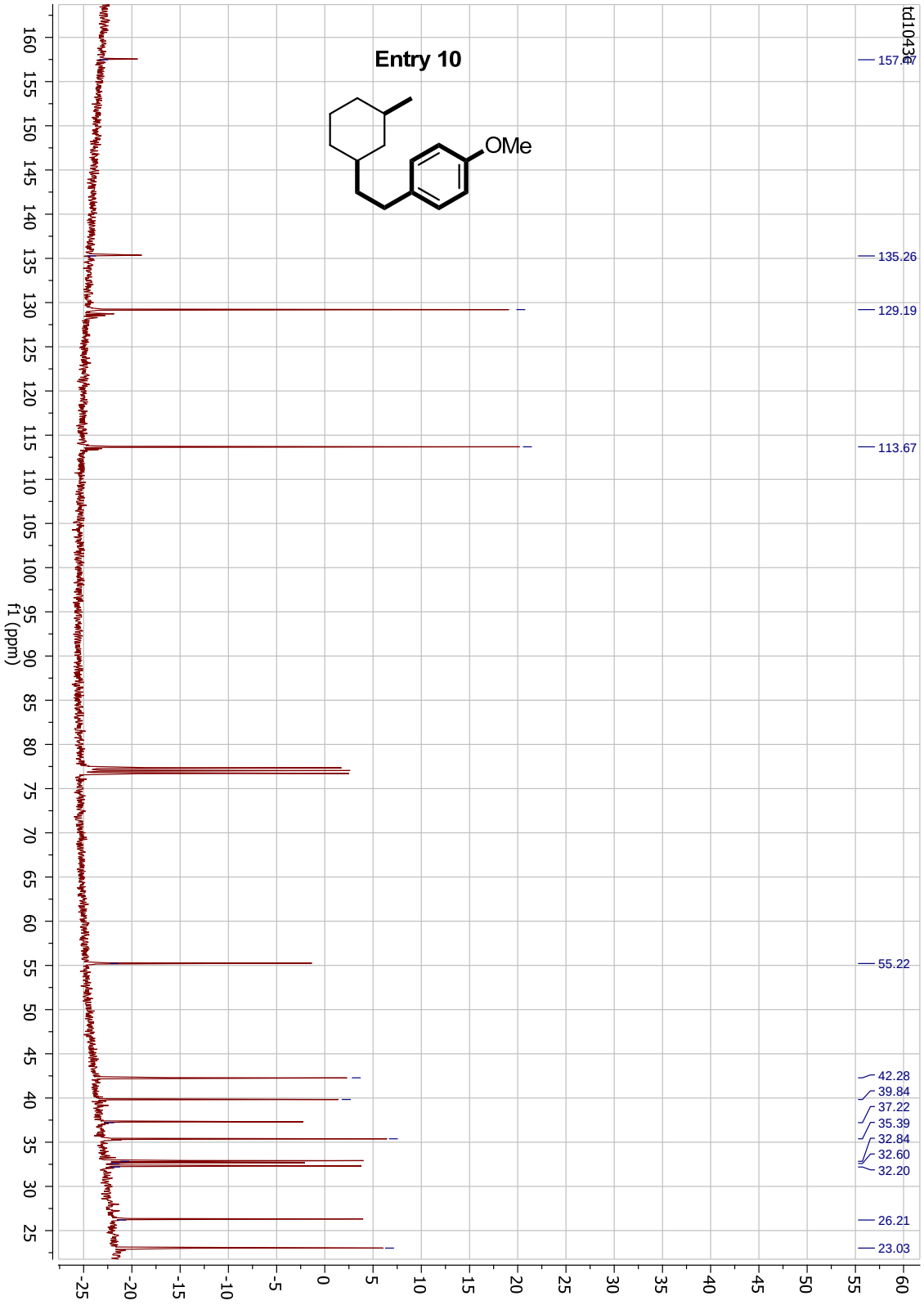
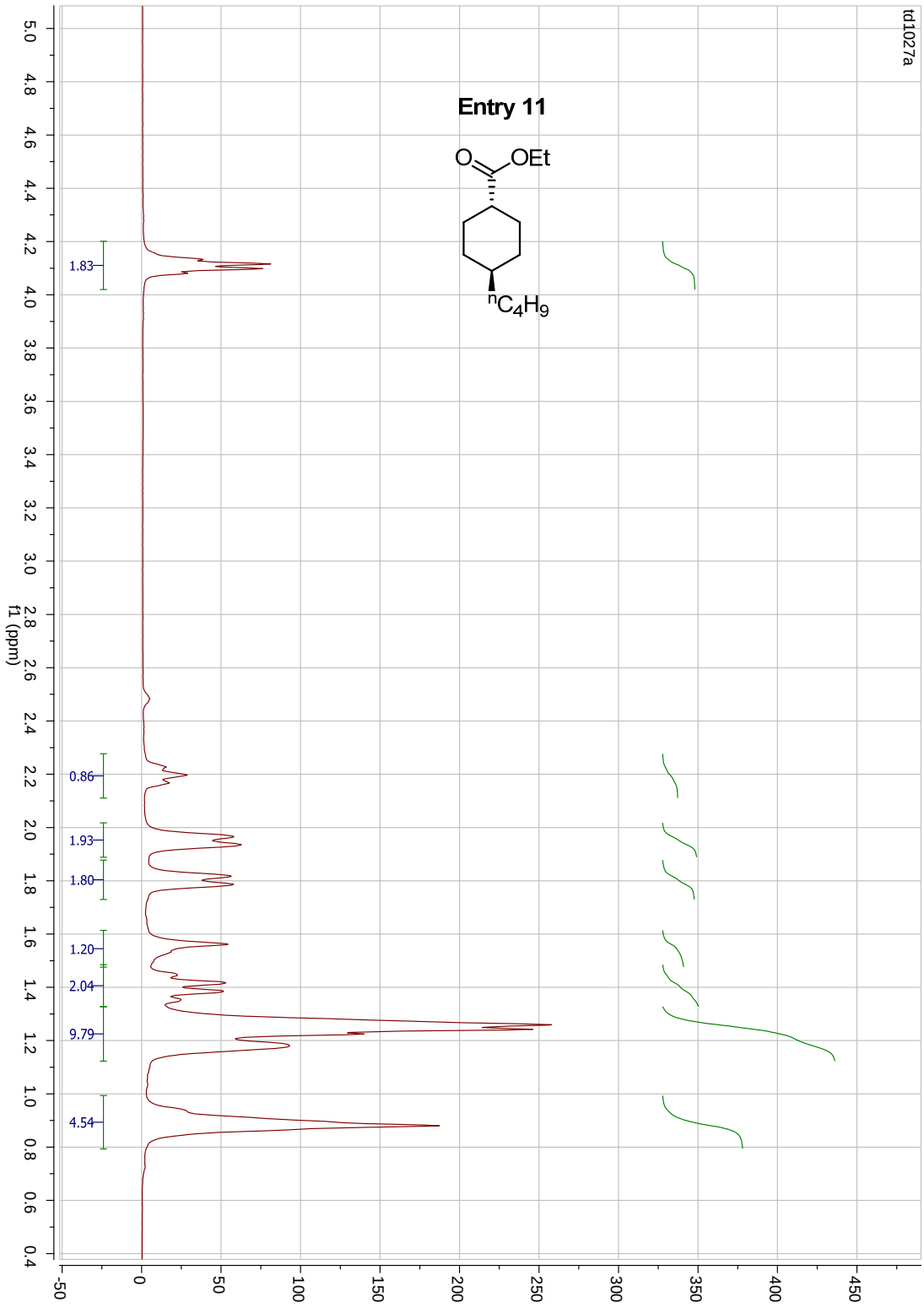
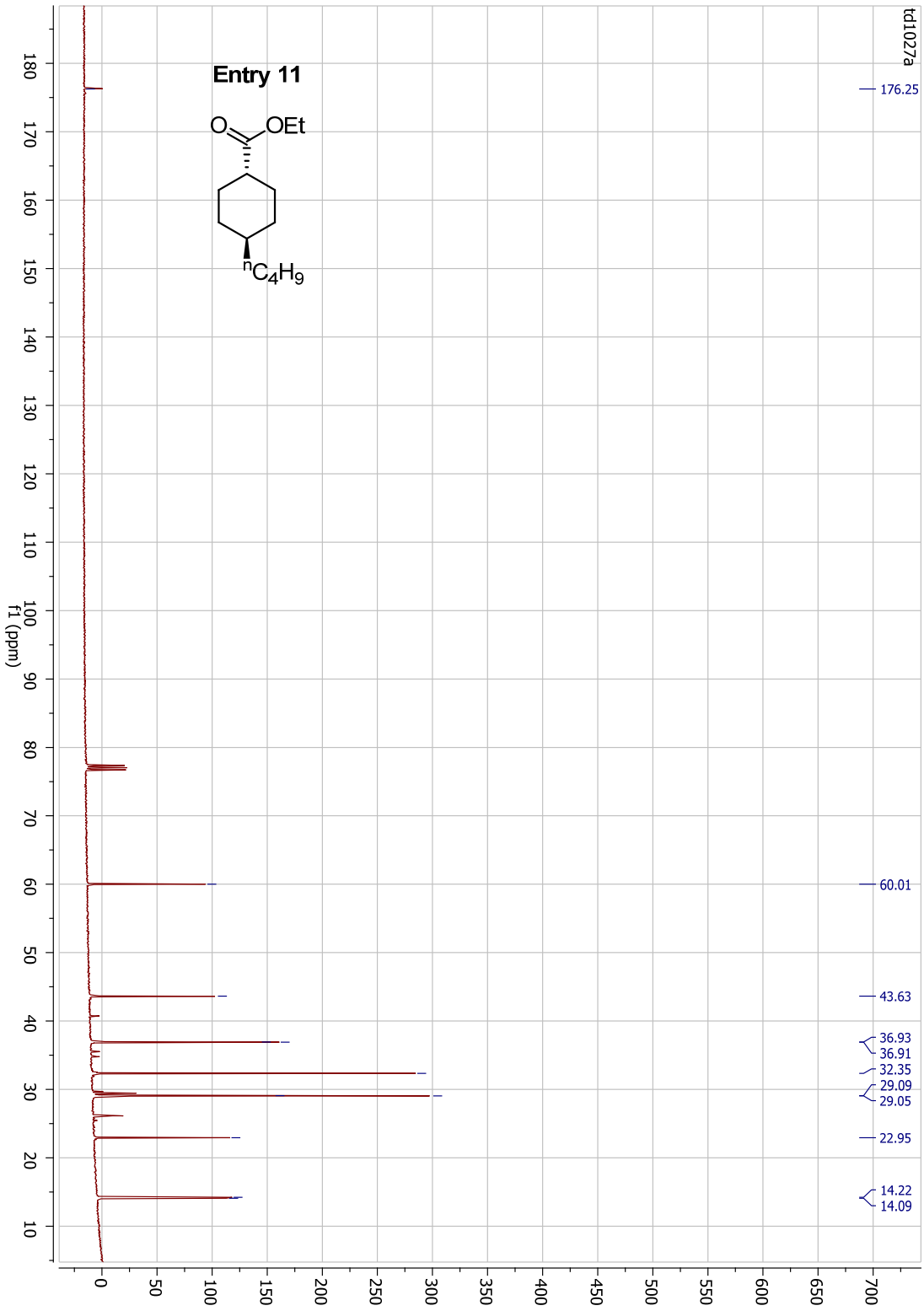
2.54
1.80
4.01
2.31
3.43
5.37
0.84
f1 (ppm)

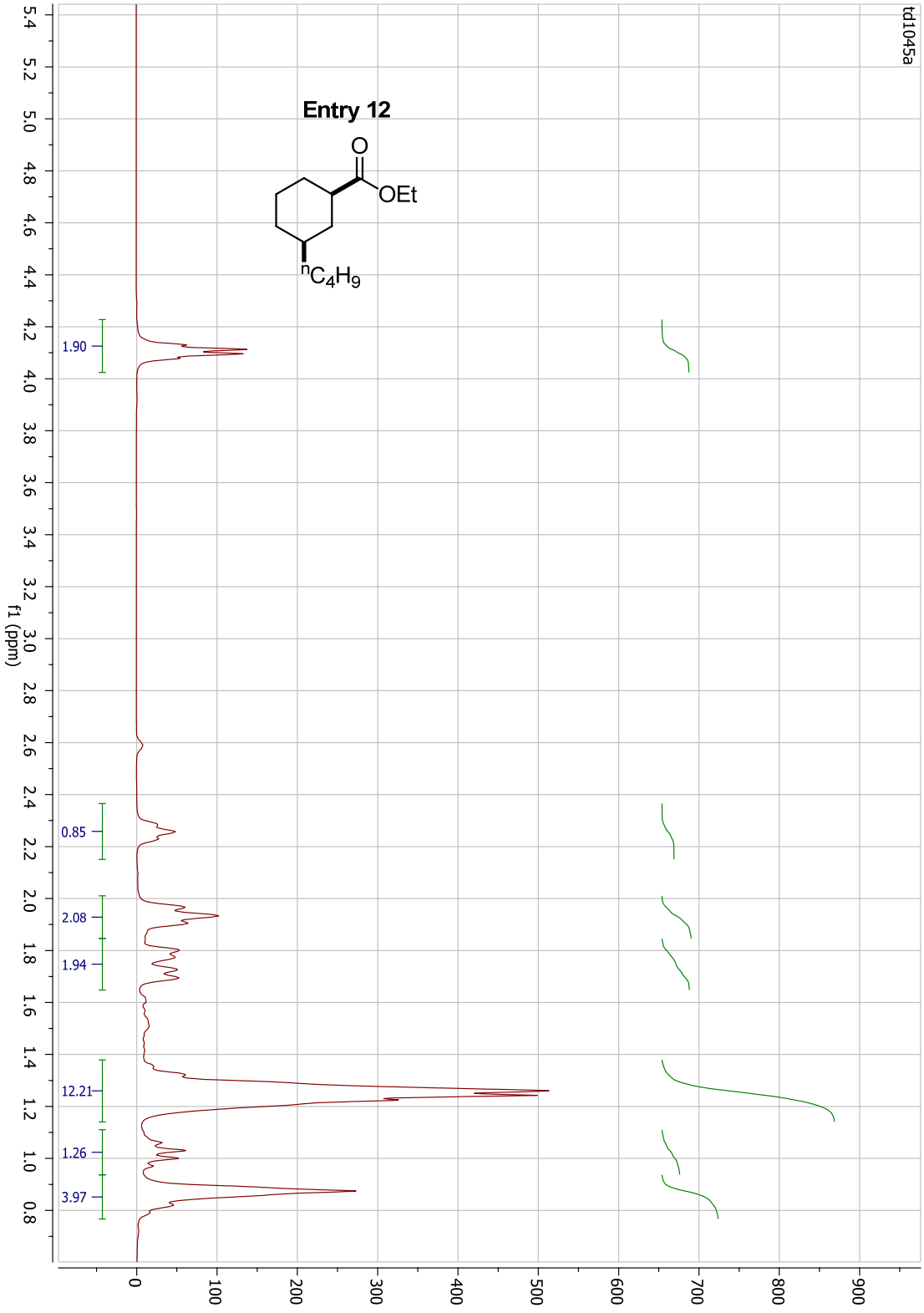

Entry 9
td1042b
143.22
128.40
128.30
125.55
42.31
39.65
37.44
35.43
33.34
32.96
32.73
26.36
23.07
f1 (ppm)

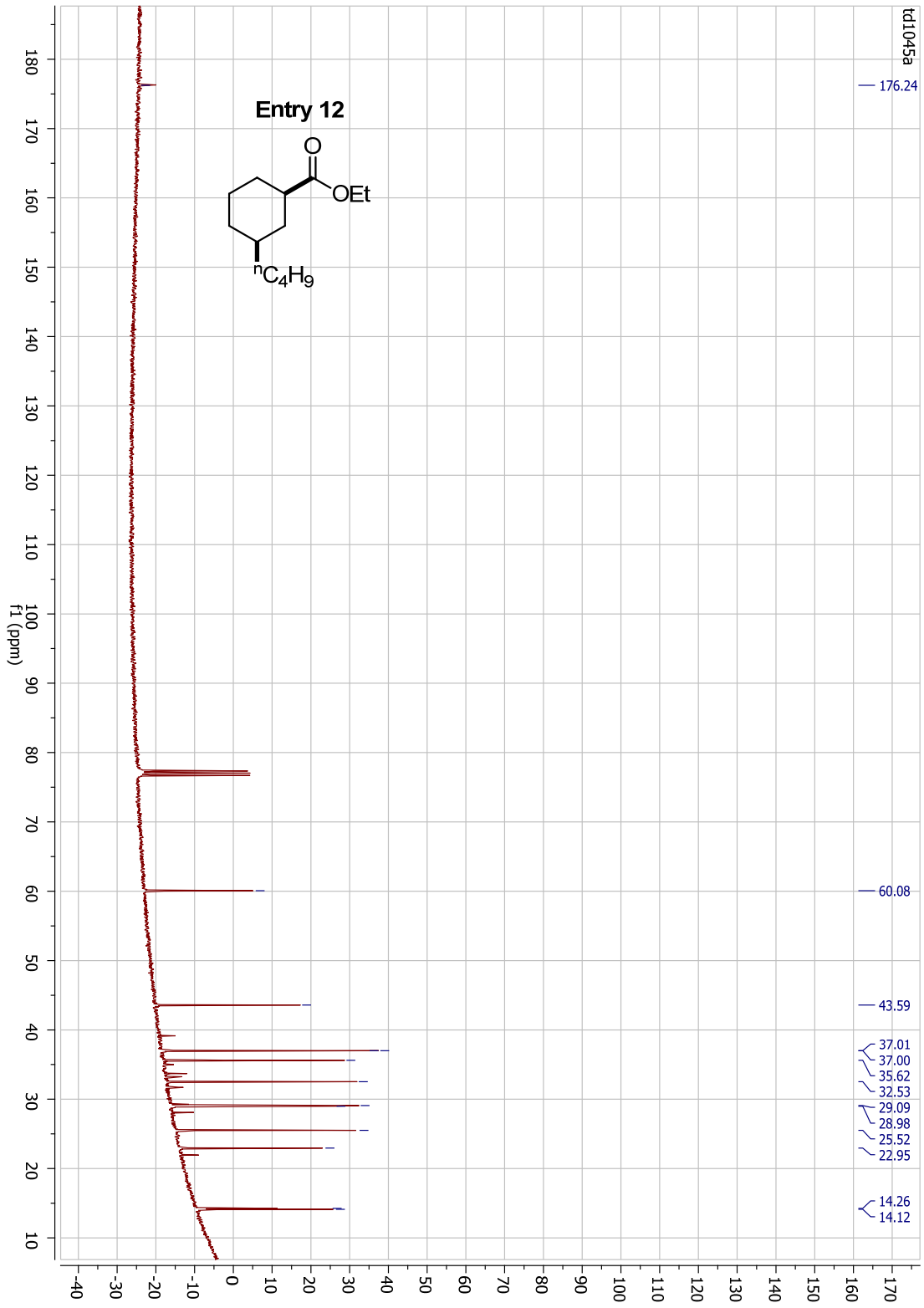

Entry 10
OMe
td1043c
f1 (ppm)
1.90
1.86
3.03
1.90
3.75
2.10
3.50
4.95
0.87

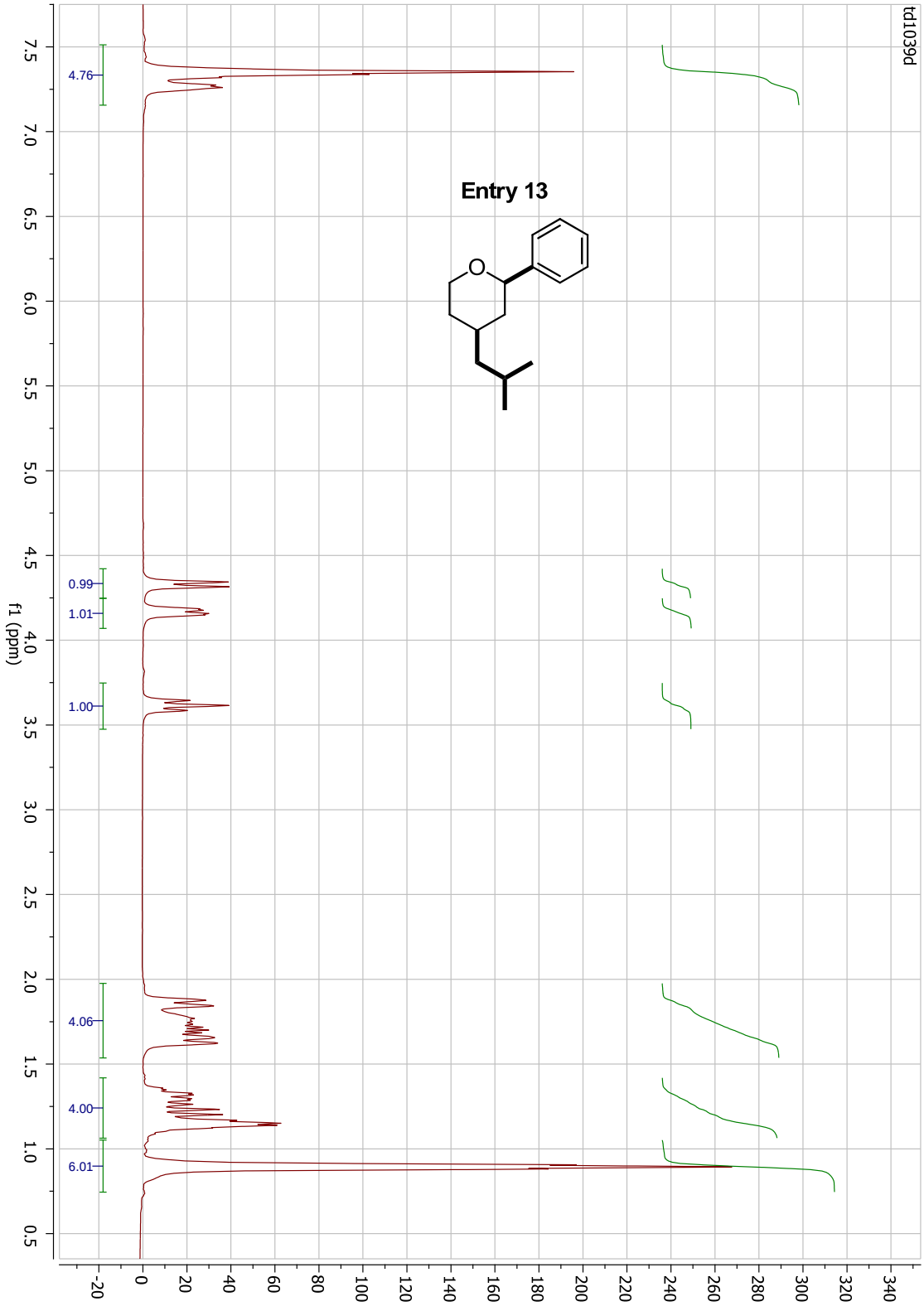

Entry 10
OMe
td10436
157.77
135.26
129.19
113.67
55.22
42.28
39.84
37.22
35.39
32.84
32.60
32.20
26.21
23.03
f1 (ppm)

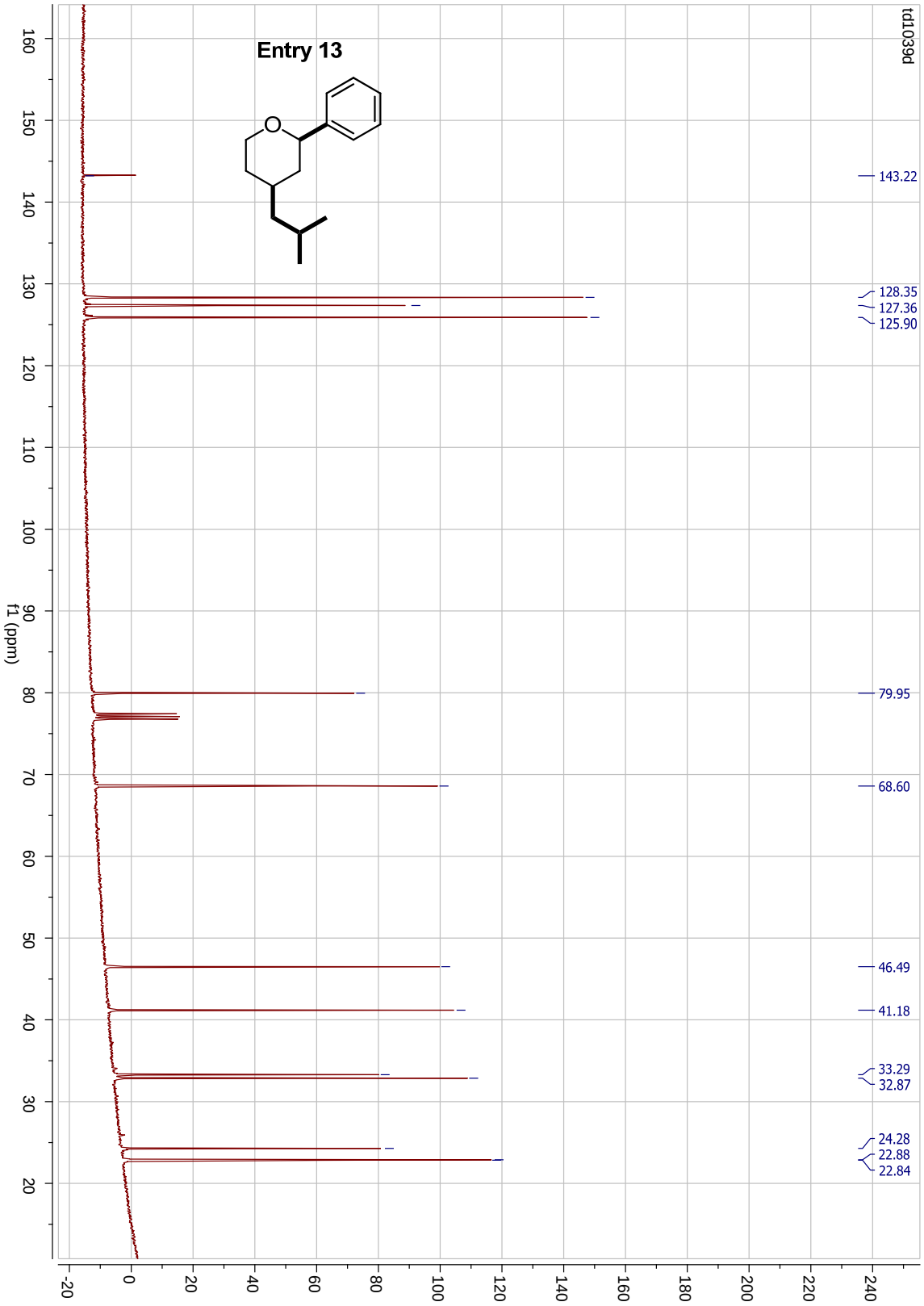

td1027a
Entry 11
O
OEt
nC4H9
1.83
0.86
1.93
1.80
1.20
2.04
9.79
4.54
f1 (ppm)

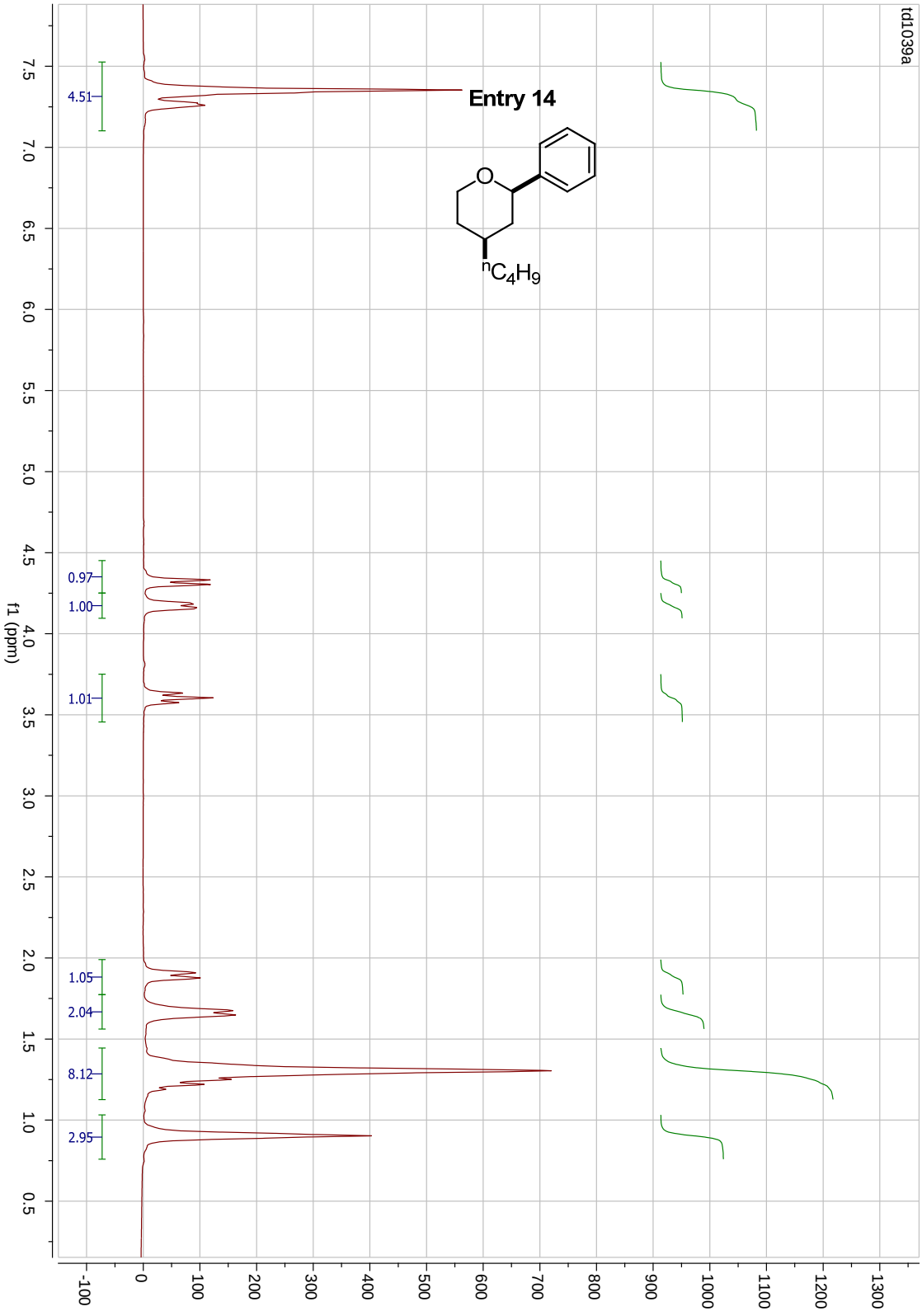

Entry 11
O
OEt
nC4H9
td1027a
176.25
60.01
43.63
36.93
36.91
32.35
29.09
29.05
22.95
14.22
14.09
f1 (ppm)

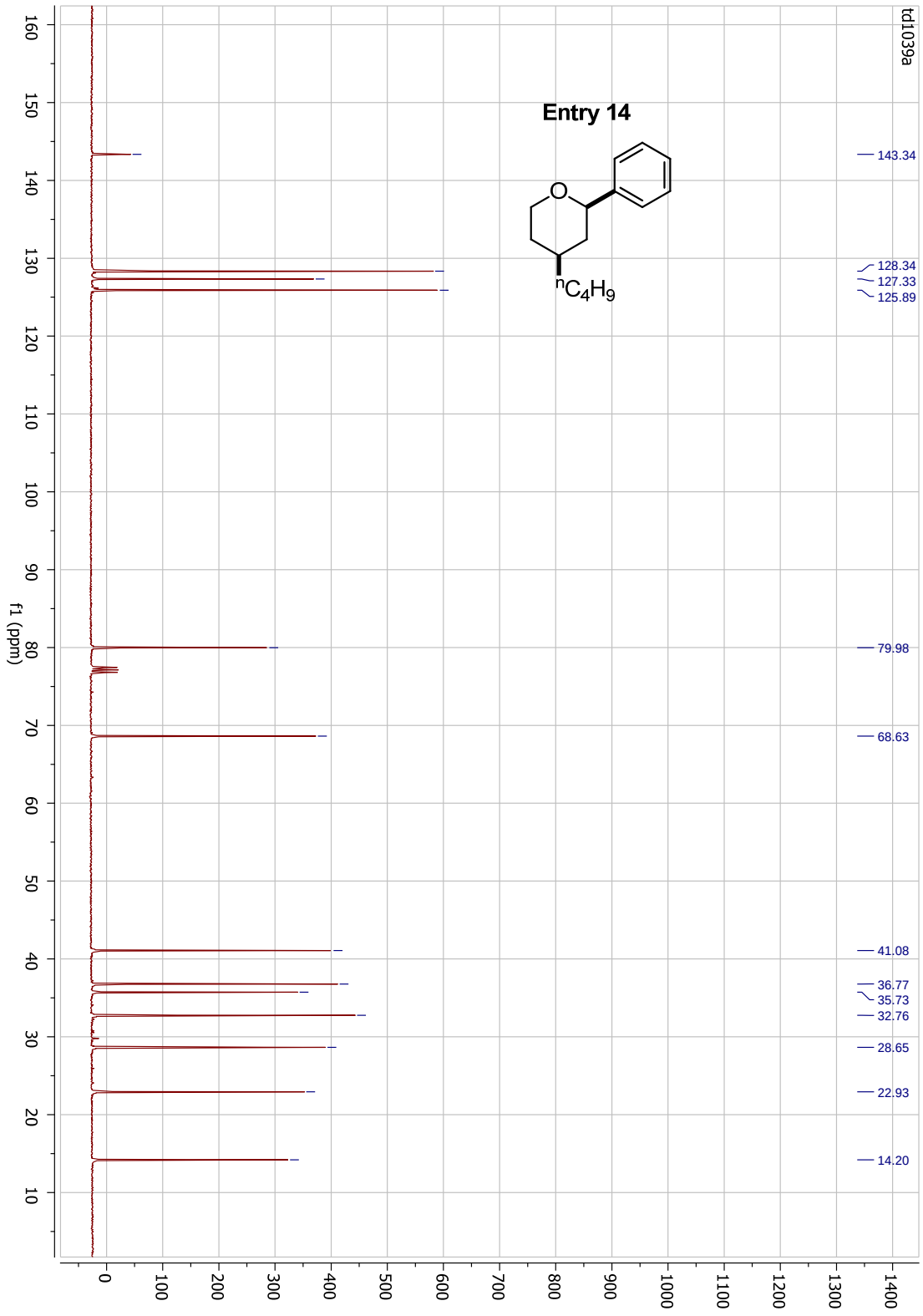

td1045a
Entry 12
O
OEt
nC4H9
1.90
0.85
2.08
1.94
12.21
1.26
3.97
f1 (ppm)


Entry 12
O
OEt
nC4H9
td1045a
176.24
60.08
43.59
37.01
37.00
35.62
32.53
29.09
28.98
25.52
22.95
14.26
14.12
f1 (ppm)

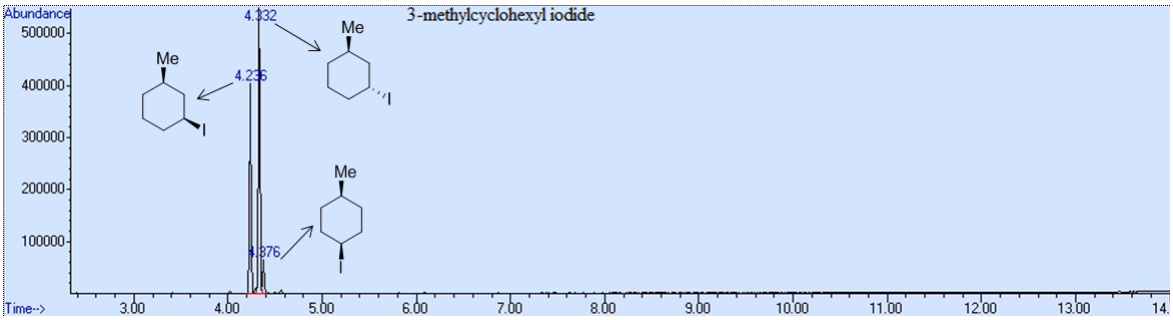

td1039d
Entry 13
O
4.76
0.99
1.01
1.00
4.06
4.00
6.01
f1 (ppm)

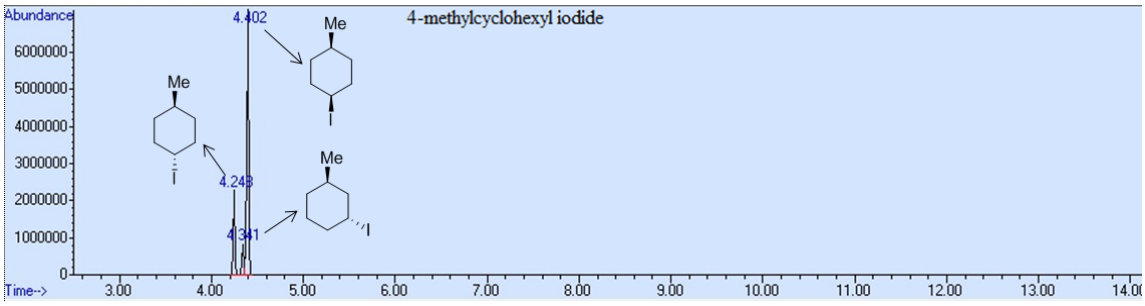

Entry 13
td1039d
143.22
128.35
127.36
125.90
79.95
68.60
46.49
41.18
33.29
32.87
24.28
22.88
22.84
f1 (ppm)

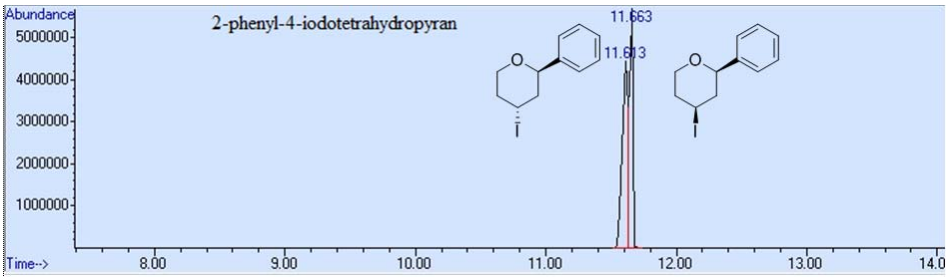

td1039a
Entry 14
O
nC4H9
4.51
0.97
1.00
1.01
1.05
2.04
8.12
2.95
f1 (ppm)

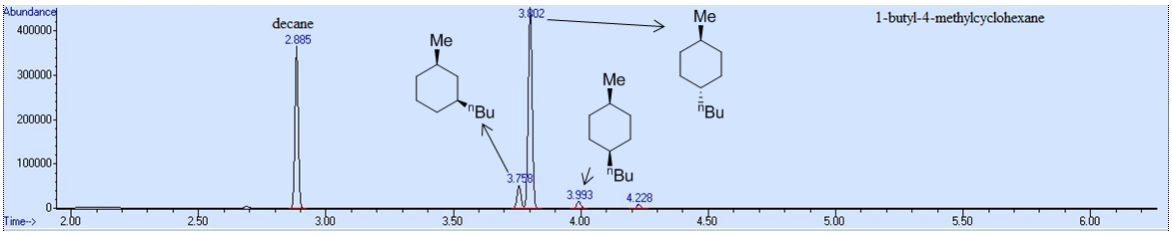

td1039a
Entry 14
O
nC4H9
143.34
128.34
127.33
125.89
79.98
68.63
41.08
36.77
35.73
32.76
28.65
22.93
14.20
f1 (ppm)

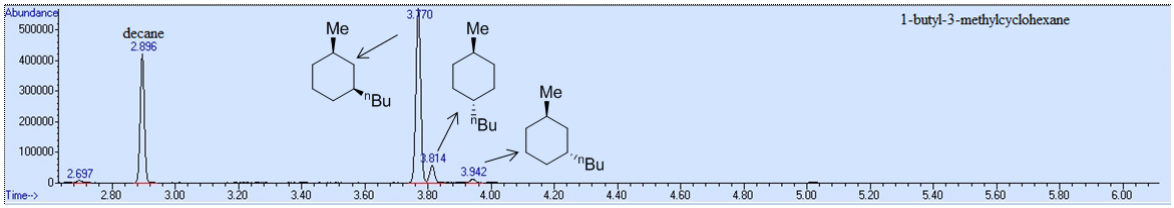
GC spectra of starting materials and products. Note that for 3-methylcyclohexyl iodide, there is a small amount of 4-methylcyclohexyl iodide present; likewise, for 4-methylcyclohexyl iodide, there is a small amount of 3-methylcyclohexyl iodide. The yields are corrected against these small impurities.










1-butyl-3-methylcyclohexane
decane
2.896
3.770
3.814
3.942
2.697

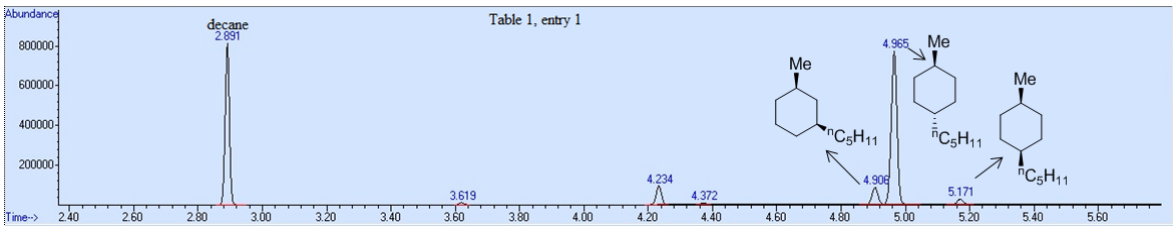


Table 1, entry 1
decane
2.891
4.965
4.906
5.171
4.234
4.372
3.619

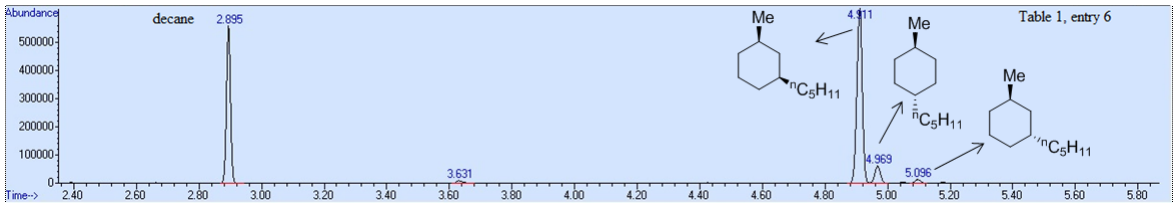


Table 1, entry 6
decane
2.895
4.911
4.969
5.096
3.631

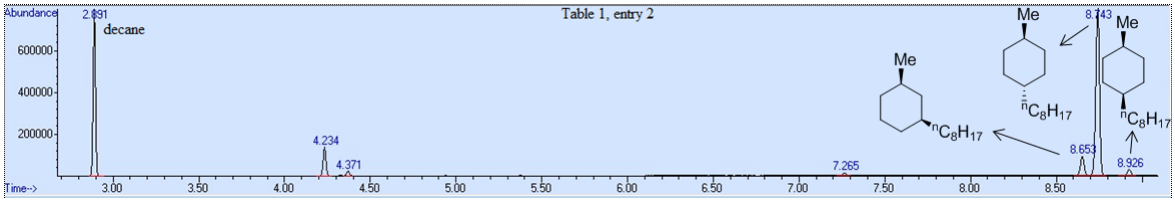
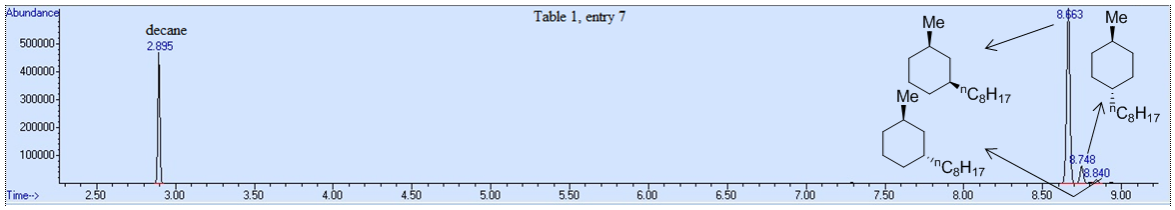


Table 1, entry 2
decane
2.891
8.743
8.653
8.926
4.234
4.371
7.265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decane
2.895
8.653
8.748
8.840

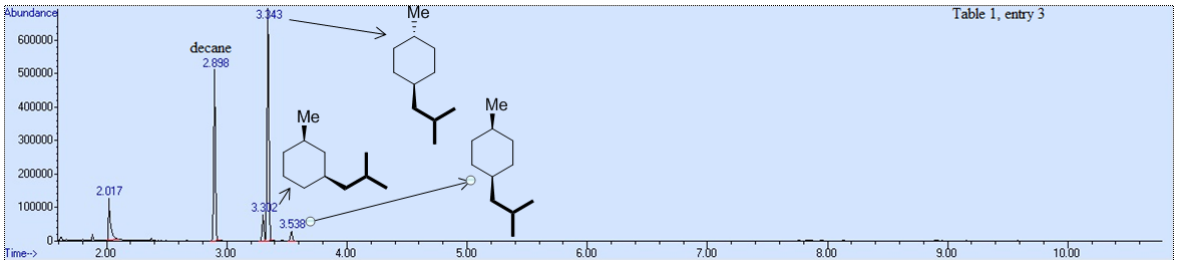
Table 1, entry 3
decane
2.898
3.343
3.302
3.538
2.017

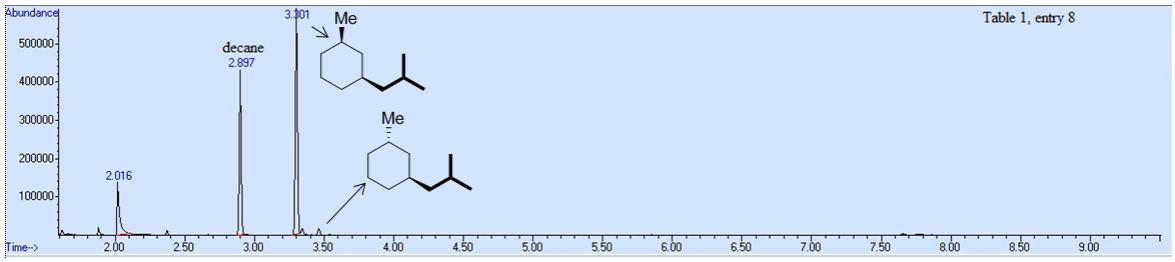
Table 1, entry 8
Abundance
decane
2.897
3.301
2.016
Me
Me
Time-->

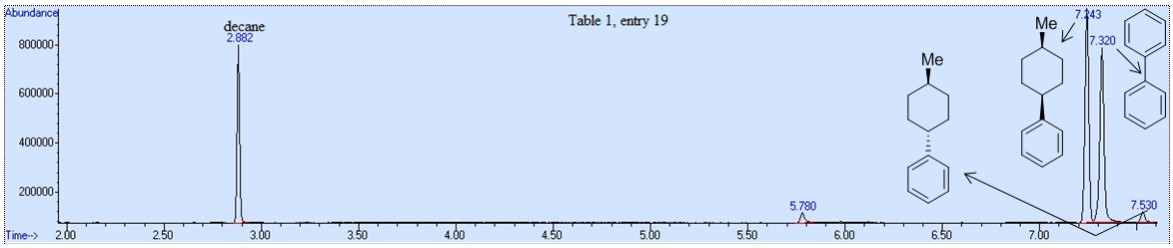
Table 1, entry 19
Abundance
decane
2.882
5.780
7.243
7.320
7.530
Me
Me
Time-->

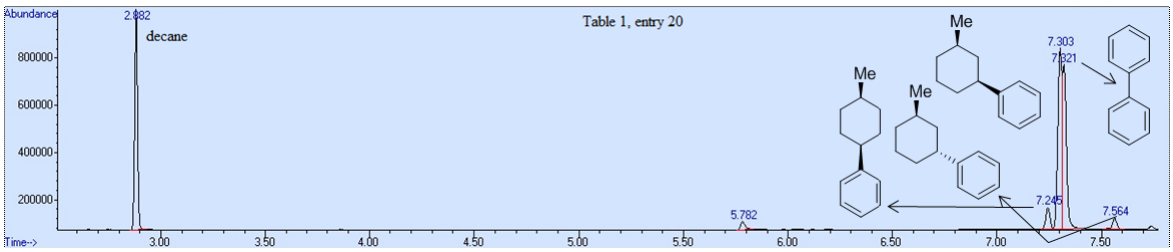
Table 1, entry 20
Abundance
2.882
decane
5.782
7.303
7.321
7.245
7.564
Me
Me
Me
Time-->

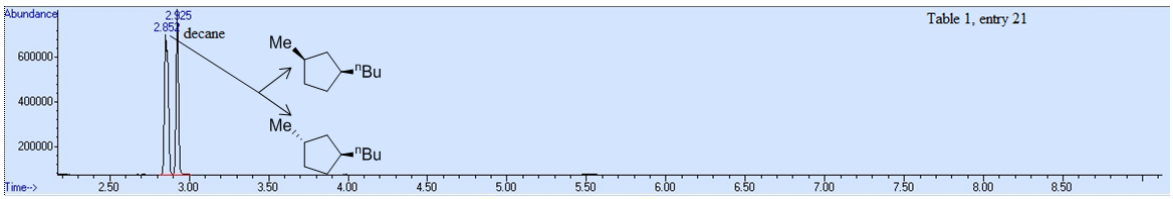
Table 1, entry 21
Abundance
2.425
2.652
decane
Me
nBu
Me
nBu
Time-->